CACHE NEWS

News about Computers in
Chemical Engineering Education

No. 51 **Fall, 2000**

CACHE NEWS

Volume 51 **Fall, 2000**

TABLE OF CONTENTS

THE CACHE CORPORATION

WHAT IS CACHE?

CACHE is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960s the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, fourteen chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. The CACHE Committee was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers including both educators and industrial members and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its ongoing projects. Information on CACHE activities is regularly disseminated through CACHE News, published twice yearly.

CACHE Trustees

Peter Bullemer
Honeywell Technology Center
peter.bullemer@honeywell.com

Edward M. Rosen
EMR Technology
edwardmemrose@cs.com

James Michaels
Merck & Company
james_michaels@merck.com

Jeffrey J. Siirola
Eastman Chemical Company
siirola@eastman.com

CACHE Task Forces and Committees

Standing Committees

Publications
Brice Carnahan **(Chair)**
Scott Fogler
Jeff Siirola

Newsletter
Scott Fogler
Peter Rony
Eddie Rosen

Conferences
Larry Biegler
Brice Carnahan
Peter Cummings
Tom Edgar
Gintaras Reklaitis
Bob Seader
Warren Seider
Jeff Siirola **(Chair)**

Industrial Trustees
Rakesh Agrawal
Edward Rosen **(Chair)**
Jeff Siirola
Peter Bullemer
James Michaels
Babatunde Ogunnaike

Task Forces

Process Engineering
Rakesh Agrawal
Larry Biegler
Michael Cutlip
Edward Rosen **(Chair)**
Bob Seader
Warren Seider
Jeff Siirola
Venkat Venkatasubramanian

Case Studies
Larry Biegler
Gintaras Reklaitis

Molecular Modeling
Peter Cummings **(Chair)**
Scott Fogler
David Kofke
Warren Seider
Venkat Venkatasubramanian
Phil Westmoreland

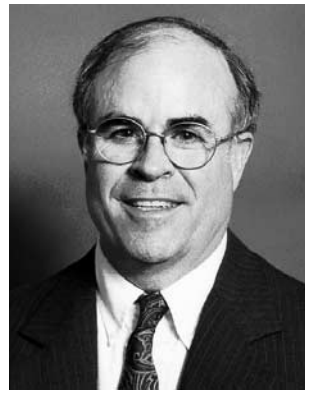
Website
Brice Carnahan
Peter Cummings
Michael Cutlip
James Davis **(co-chair)**
Frank Doyle **(co-chair)**
Thomas Edgar
Scott Fogler
Peter Rony
Bob Seader

Industrial Affiliates

AEA/Hyprotech
Air Products and Chemicals, Inc.
Aspen Technology
DuPont
Eastman Chemical Company
ExxonMobil
Equilon
Inst. Mexicano del Petroleo
Merck & Co. Inc.
Pfizer/Parke Davis
Union Carbide Corporation

New Executive Officer

Tom Edgar
The University of Texas at Austin



After 16 years of service Professor David Himmelblau is stepping down as Executive Officer of the CACHE Corporation, although he will remain a Trustee of CACHE. The Trustees held a recognition dinner for David last year and presented him with a plaque which said "With special thanks and appreciation for his dedication, leadership, and many years of service as Executive Officer". The CACHE office will remain in Austin, Texas. Effective July 1, 2000 Professor Tom Edgar assumed the role of Executive Officer for the next two years. Tom is well-known in the chemical engineering education and computing communities through his textbooks, education lectures, and research in process modeling and control. Having had a number of administrative positions at UT-Austin as well as leading several professional organizations, Tom understands what is needed to keep the office running smoothly and responsive to customer needs. He has also had considerate involvement with CACHE conferences as an attendee as well as on organizing committees.

New CACHE Trustee

Peter Bullemer
Honeywell Laboratories

Peter Bullemer is a research and technology program manager at Honeywell Laboratories. He received a B.A. in Psychology (1976) and Ph.D. in Experimental Psychology (1988) from the University of Minnesota. Involved in Honeywell corporate research and development since 1987, Dr. Bullemer has extensive programmatic and technical leadership experience in research and development of training, information and decision aiding technologies for human operators in complex interaction environments. He is a founder and visionary of a multiyear effort to understand and improve abnormal situation management practices in industrial process control industry. He initiated the Abnormal Situation Management program in 1993 as a series of extensive field studies within the plant setting to characterize the nature of the problem, define short- and long-term solution requirements, and develop an R&D roadmap. The initial phase results were instrumental in forming the Abnormal Situation Management (ASM) Joint R&D Consortium in 1994. In 1995, Dr. Bullemer was the principal investigator with overall technical lead responsibility, on a 3.5-year, $16.6 million cooperative agreement grant from NIST ATP program, *Collaborative Decision Support for Industrial Process Control*. In this role, he led the definition of technical scope and integration of technical developments in intelligent software architecture, process diagnostics, dynamic planning and user interface design of a collaborative decision support prototype.

Dr. Bullemer is the current program manager and principal investigator of the ASM Consortium's new three-year program (1999-2001) to transition the technical innovations of the NIST program into product development. Key objectives of this program include demonstrating feasibility of the solution concepts in the operational environment, initiating product development interest, informing product development organizations of the solution requirements, and consulting with applications developers in the operational setting. His current research interests include:

- Impact of culture and organizational practices on the effective use of technology
- Design of human-system interaction to improve human performance and learning
- Development of human-centered systems engineering methodologies

New CACHE Trustee

James N. Michaels
Merck & Co. Inc.

Dr. Michaels received his B.S. and M.S. in Chemical Engineering from the University of California at Berkeley in 1977, a Diploma in Physical Chemistry from Imperial College, London in 1978, and an Sc.D. in Chemical Engineering from M.I.T. in 1983. He joined the Chemical Engineering faculty at U.C. Berkeley in 1984 where his research program focused on atomic mobility in the solid-state with application to catalysis and solid-oxide electrochemical cells. In 1990, he joined the Central Research Laboratory of Mobil Research and Development Corporation where he worked on projects ranging from oxidation catalysis to oil reservoir wettability. In 1993, Dr. Michaels joined the Manufacturing Division of Merck & Co., Inc., where he established a particle technology group that supports R&D and global technical services groups in the transfer of new products into manufacturing and troubleshooting of pharmaceutical products and processes.

New CACHE Trustee

Babatunde A. Ogunnaike
DuPont

Babatunde A. ("Tunde") Ogunnaike received his B.S. degree in Chemical Engineering from the University of Lagos, Nigeria, in 1976; the M.S. degree in Statistics, and the Ph.D. degree in Chemical Engineering (specializing in Process Control) from the University of Wisconsin-Madison, both in 1981. From 1981-1982 he was a Research Engineer with the Process Control group of the Shell Development Corporation in Houston, Texas; from 1982 to 1988 he was a professor at the University of Lagos, Nigeria, with joint appointments in Chemical Engineering and Statistics. He joined the Advanced Control and Modeling group at DuPont in 1989 where he is currently a Research Fellow. He has also been an adjunct professor in Chemical Engineering Department of the University of Delaware since 1989. He is currently an Associate Editor of the journal "Industrial and Engineering Chemistry Research". His research interests include identification and control of nonlinear systems, modeling and control of polymer reactors and distillation columns, implications of design on process controllability, design of inherently robust processes, applied statistics, and reverse engineering biological control systems for process applications. He remains very active in the COMPUTERS AND SYSTEMS TECHNOLOGY (CAST) Division of the American Institute of Chemical Engineers (AIChE).

Introduction to This Issue

Edward Rosen, Scott Fogler and Peter Rony

CACHE News, No. 51 (Fall 2000), is the first online issue of the CACHE Corporation newsletter. It will join back issues of the newsletter that can be accessed at the CACHE website http://www.CACHE.org/. The last printed issue was No. 50 (Spring 2000).

By going online, we -- members of the CACHE Newsletter Committee -- hope that CACHE News will become more accessible to chemical engineering faculty, students, and professionals. Each article can be downloaded separately so that a single, large file for an online issue need not be acquired.

By going online, we provide opportunities for our authors to incorporate color and color images, provide animations (e.g., the results of computational fluid dynamics (CFD) computations), streaming audio, and streaming video as an expanded set of data structures.

CACHE News encourages contributions that are both useful and reflect the latest experience or thinking in the interface between chemical engineering and computing in the educational arena. The author of any article retains copyright ownership, and can submit it later to a peer-reviewed journal. Submitted articles are scanned for appropriateness by the co-editors but are not peer reviewed.

We specially encourage submissions that probe new directions in chemical engineering education. Three examples of such articles in issue No. 51 are "Engineering and Computational Issues in Industrial Biology", by Babatunde Ogunnaike, "Chemical Microengineering. I. Introduction", by Peter Rony, and "The Interactive Authorship", by James Riggs. In this way we hope that CACHE News will beneficially influence the evolution of the chemical engineering curriculum.

CACHE Newsletter Committee,

Edward Rosen
Scott Fogler
Peter Rony

CACHE Website
Soliciting Educational Materials

Thomas F. Edgar

CACHE has recently redesigned its website to give it the modern look and feel of a modern portal, serving a learning community made up of chemical engineering faculty and students. During the past year www.cache.org has been continually adding new features, especially in the Teaching Resource Center.

The Teaching Resource Center provides educational materials from faculty, such as syllabi for different courses, software, simulation, and text material. There also is an online directory of all chemical engineering faculty. We are requesting faculty to put links to their materials on the CACHE web page, since search engines are often unable to identify relevant information. The first fully developed prototype has been developed by Tom Edgar in the area of process control. Other areas to be covered include:

Introduction to Chemical Engineering
Material and Energy Balances
Mass Transfer
Heat Transfer
Fluid Mechanics
Thermodynamics
Transport Phenomena
Separation Processes
Unit Operations
Kinetics and Reaction Engineering
Process Control
Numerical Methods
Process Design
Material Science
Catalysis
Pollution Control
Hazardous Waste Management
Polymer Science
Molecular Simulation

Technical Communication

There are other curriculum areas with good content in them, notably Molecular Simulation and Process Design.

Frank Doyle and Jim Davis are now chairing this project. They will be identifying area editors for the above curriculum topics to moderate each area. Faculty who would like to volunteer to moderate a given area should contact Frank Doyle at fdoyle@udel.edu.

Brice Carnahan's

Predictions on Information Technology

J.D. Seader

It is an honor for me to have the opportunity to spend a few minutes to talk about the accomplishments of Brice Carnahan.

I first became acquainted with Brice in the mid-1960s, after he had completed a PhD in chemical engineering at the University of Michigan, where he had been one the main driving forces in the Ford Foundation and NSF projects, under the leadership of Don Katz, to study the use of computers in engineering education. Those groundbreaking projects set a direction for Brice that has continued to the present time.

Since the mid-1960s, I have had the pleasure of associating with Brice mainly through the CACHE organization and I would like to direct my comments mainly to his endeavors with CACHE. However, before I begin those comments, I would like to mention two accomplishments outside of CACHE that have impressed me greatly:

1. The textbook, "Applied Numerical Methods", which he co-authored with Luther and Wilkes in 1969. This book, which was dedicated to Don Katz, is still very useful and is a model of theory and application.

2. The "Computing in Chemical Engineering Award" of the CAST Division of AIChE, which he received in 1980. He was the second person to receive that award.

In April of 1969, Brice, together with Warren Seider and Rudy Motard, organized a meeting of chemical engineering educators interested in computing. This meeting led to the formation of the CACHE Committee, in November of that year, 31 years ago. Brice was selected as the first Chairperson of CACHE and has been an active member of CACHE ever since. His first task was to obtain initial funding from NSF, which he accomplished.

During his early association with CACHE, Brice became the leading expert among chemical engineers in FORTRAN programming style and documentation. His program, GOLDEN, served as a model for others to follow. Brice's interest in the numerical solution of ODEs, led him to develop one of the first dynamic simulation programs, DYSCO. In the early 1980s, Monsanto gave permission to CACHE to prepare load modules for all of the popular computers from the FORTRAN source code for their steady-state simulator, FLOWTRAN. Brice prepared the first load module, with detailed documentation of how he did it so that the development of load modules by other educators for 13 other computers would be facilitated.

In 1974, Brice assumed the responsibility for editing, printing, and distributing CACHE publications. He has continued with this responsibility for the last 26 years, During that time, he has distributed more than 20 different CACHE publications, including 15,000 copies of the FLOWTRAN books.

Brice was one the first chemical engineering educators to recognize the potential of the PC. In 1978, Brice, together with Scott Fogler, took the leadership in the use of PCs for education and obtained a significant NSF grant, which included the development of an authoring program. I still remember the first time I saw an IBM PC. Brice had it and demonstrated it to me. I remember asking him, when the A: \ appeared on the screen, "Now what do you do?"

In 1996, in connection with the 25th anniversary of CACHE, Brice edited, published, and distributed the volume, "Computers in Chemical Engineering Education", consisting of 20 solicited papers by 35 authors. The last paper, entitled "2001", was written by Brice. His paper was a short review of computing and a set of predictions for 5 years into the future. The final sentence of his paper was, "The conjectures about the future are largely my own; fortunately, I can't be proved wrong until 2001,….", Well, 2001 is almost here. Let's see how some of the predictions of Brice have turned out:

1. Yes, Moore's law continues to hold.

2. Yes, the operating system is largely integrated with the worldwide web.

3. Yes, chemical engineering students are largely being taught high-level languages rather than FORTRAN and C.

4. Yes, JAVA has become a predominant operating system because of its cross-platform compatibility.

5. Yes, many educators have web home pages and information links for their

courses.

6. Yes, the worldwide web allows universities to keep in touch with and deliver continuing education courses to their alumni.

Chemical engineering educators have been greatly benefited by the vision and efforts of Brice Carnahan during the past 40 years. It has been an honor for me to know him and to associate with him.

Editor's note: The 1996 paper by Brice Carnahan is included in this issue of CACHE News.

2001

Brice Carnahan
University of Michigan
Ann Arbor, MI 49109

Abstract

1996 is a special year in the history of computing. It marks the 50th anniversary of the public announcement of the ENIAC, the first general-purpose electronic digital computer, the 25th anniversary of the first commercial microprocessor, the Intel 4004, and the 15th anniversary of the first IBM PC, whose basic structure and open architecture set the standard for subsequent personal computer development.

Most technological developments of consequence pass through the familiar S curve of slow initial growth, then a period of rapid acceleration, and finally another slow-growth phase of important, but marginal, improvement. For the digital computer, the slow growth period lasted about 15 years. The acceleration phase began with the introduction of the transistor in the late 1950s, received additional thrust with each new transforming technology (time-sharing, integrated circuits, real-time minicomputers, networking, the microprocessor, interactive graphical operating systems and programming environments, supercomputers and parallel machines, high speed communications, the Internet, the World Wide Web, etc.), and continues unabated to this day.

We describe past developments and current trends in the areas of computing hardware, communication, and software and make a few predictions about the state of computing in general and in chemical engineering education in the year 2001.

Introduction

Only "yesterday" those two most prominent dates of 20th century fiction, Orwell's *1984* and Clark's *2001*, seemed far into the future. Today, 1984 (do you remember your IBM PC AT or Macintosh 128?) is long past, and Big Brother is (almost) nowhere in sight.

2001 looms over the horizon, a mere half-decade away. And Clark's HAL, malevolent and almost infallible, also seems nowhere in sight. But, of course, he won't be "born" until 1997, so there is still time! One certainty is that HAL will look nothing like Kubric's 1969 vision of him. No astronaut in full space suit will float among HAL's innards. More likely, all of HAL's parallel processing capability will be encompassed in many microprocessors, housed in a "box" of quite modest size.

Neither Orwell nor Clark should be faulted for his vision. Predictions about the future of technology have not been particularly accurate. Verne was right about moon travel, and in his 1863 novel *Paris in the Twentieth Century* correctly imagined the automobile, electric lights, and the fax machine, but was wrong about many others. Edward Tenner, in his recent *Why Things Bite Back,* argues convincingly that most predictions about technological developments turn out to be either off the mark or just dead wrong.

Two of my favorite predictions, both from Vannevar Bush (inventor of the analog computer and World War II production czar), show how long-term right and short-term wrong the *same* person can be about the *same* subject:

> " ... The MEMEX will be for individual use, about the size of a desk with display and keyboard that will allow quick reference to private records, journal articles and newspapers, and perform calculations ..."
>
> in *As We May Think* (1945)
>
> " ... Will we soon have a personal machine for our own use? Unfortunately not!"
>
> in *MEMEX Revisited* (1967)

Incidentally, Bush, a consultant for IBM, is reputed to have told the IBM Board in 1955 that no more than 100 IBM 650s should be built, since they could do all the computing that the World needed done!

Even short-term prediction is fraught with peril. Few would have predicted in 1993 that a hyperlinked World Wide Web would transform computing from a machine-centered view to a network-centered one almost overnight. Despite such revolutionary surprises, technology instills a sense of unfolding promise, making prediction almost impossible to resist. Hence my title, *2001* (granted, I'm not looking all *that* far into the future!).

Hardware

Hennesey and Patterson, in their superb 1995 text *Computer Architecture* (a must-read for anyone interested in low-level computer structure and functionality), briefly outline the history of computer hardware and architectural development, noting that a 1995 desktop PC (costing say $4,000 in 1995 dollars) had more main and disk memory, and better performance, than a million-dollar (1965 dollars) 1965 main-frame.

Processors and Memory

During the twenty five years following ENIAC, actual computer "performance" (Hennesey and Patterson), a rough measure of ability to process a comprehensive mixed set of test programs, improved by about 25% per year for main-frames, year in and year out. That rate improved to between 25% and 30% during the 1970s, primarily because of the introduction of minicomputers into the hardware mix. Since 1980, following widespread production of microprocessors, the overall performance growth rate has climbed to roughly 35% per year. The Intel CISC (complex instruction set computer) microprocessor family, used in perhaps 85 percent of the approximately 75 million machines that will be sold worldwide in 1996, is primarily responsible for this acceleration in average performance.

RISC (reduced instruction set computer) processors were first introduced in 1984. Since then, overall performance of computers incorporating this class of processors has improved at about a 50% annual rate. Although used in only 10 to 15 percent of computers in the current market, RISC processors play a significant role in engineering computing, since they are used primarily in high-performance engineering workstations and parallel machines (also in Power Macintoshes).

Figure 1 (data from URL *infopad.eecs.Berkeley.edu/CIC*) shows that raw peak processor capability (rather than observed average performance for assembled computers), estimated roughly as proportional to the product of processor transistor count and clock speed, has doubled about every eighteen months over a 20 year period for the Intel family of CISC microprocessors. The Power PC and DEC Alpha RISC microprocessor families show even shorter peak performance doubling times of 12 to 14 months.

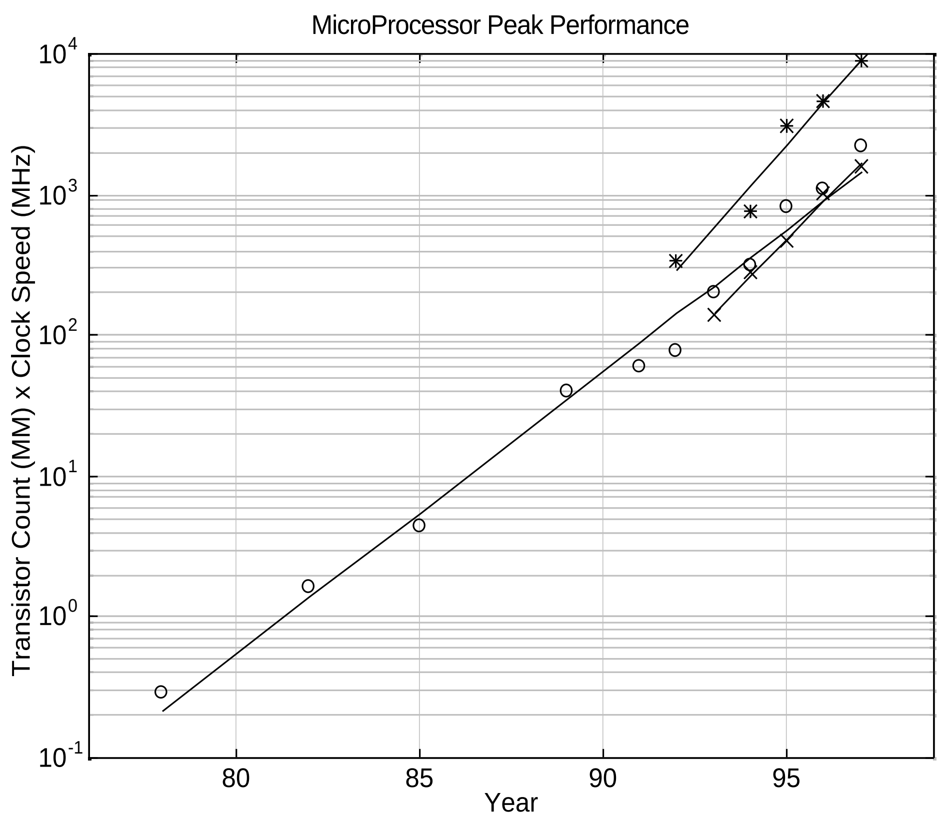


Figure 1. Peak performance estimated from the product of transistor count and clock speed for Intel (o), Power PC (x) and DEC Alpha (*) microprocessors.

Three current trends in chip and magnetic disk technologies are (Hennesey and Patterson):

1. Transistor density for integrated circuit logic (microprocessors) is increasing at about 50% per year; growth rates in transistor count per chip are in the range 60% - 80% per year.

2. Dynamic (main memory) RAM bit density is increasing at about 60% per year, resulting both from higher transistor densities and design improvements requiring fewer transistors per memory cell. The result is RAM of much larger capacity and much lower cost than was available even two or three years ago. 16 Mb chips are now standard, and 32 Mb and 64 Mb chips are widely available. [NEC has recently reported development of an experimental 4 Gbit RAM chip (256 times the capacity of the current standard chip), with production planned for around 2005.]

3. Prior to 1990, magnetic disk densities increased at about 25% per year. Since 1990, the rate has accelerated significantly to about 50% per year.

What about costs? Here, the impact of the technical developments alluded to in the preceding paragraphs, improved manufacturing performance (yield of good chips), and economies of scale resulting from volume production and commoditization of microcomputers, have led to incredible reductions in the cost/performance ratio.

Figure 2 shows a retail price curve for 16 Mb DRAM (dynamic RAM) chips between 1993 and 1996. The cost reduction by a factor of 8 to 10 over the 3 to 4 year life cycle of this DRAM chip is typical of that for prior standard chip sizes as well. With the compounding of cost reductions for standard chips, the cost per megabyte of DRAM has dropped incredibly from over $17,500 in 1977 to about $5 in 1996 (both in 1996 dollars). Thus real RAM costs have been reduced by a factor of 3500 in about 20 years!

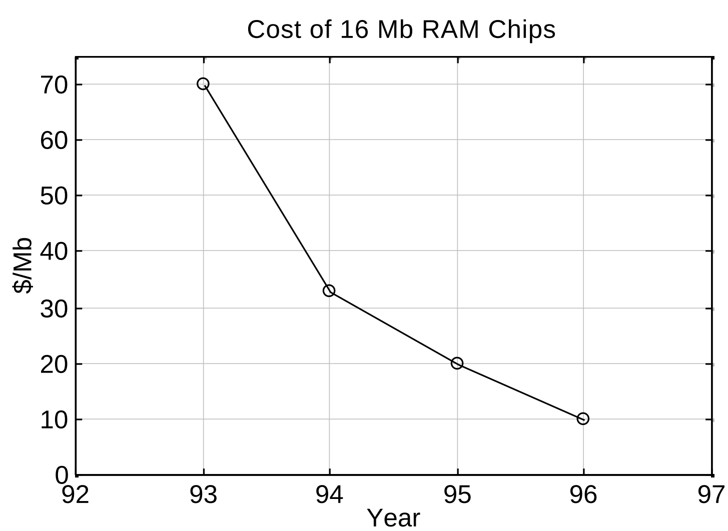


Figure 2. Cost of 16 Mb RAM chips - 8 required for 16 MB (data from Hennesey and Patterson).

What are the prospects for continuation of the performance trends for processor and memory chips described above? Very good, at least until 2001 and probably for several years beyond. Processor chips with a billion transistors and memory chips with many billions of transistors are certain to appear before the end of the first decade of the next millennium.

However, physical limitations of current photolithographic processes will force major changes in chip production technology before then. As shown in Fig. 3, the minimum feature size (e.g., width of “wire” traces) of chip-making photolithographic processes on silicon has fallen from 12 microns in 1970 to 3.5 microns in 1980 to 0.8 microns in 1990 to 0.3 microns in 1996; at least two new 0.25 micron fabrication facilities will be in full production by mid-1997. The apparent limit of this technology, 0.365 microns, the wavelength of the ultraviolet light currently used for photoresist exposure, will in fact be reduced by more than half, to 0.1 microns, with lasers emitting 0.248 micron or 0.193 micron ultraviolet light and clever use of phase-shifted interference lithography. However, barring some even more clever (and unlikely) improvement within the next very few years, the minimum feature size of photolithographic technology is probably about 0.1 microns, likely to be in common use during the first half of the next decade (Stix).

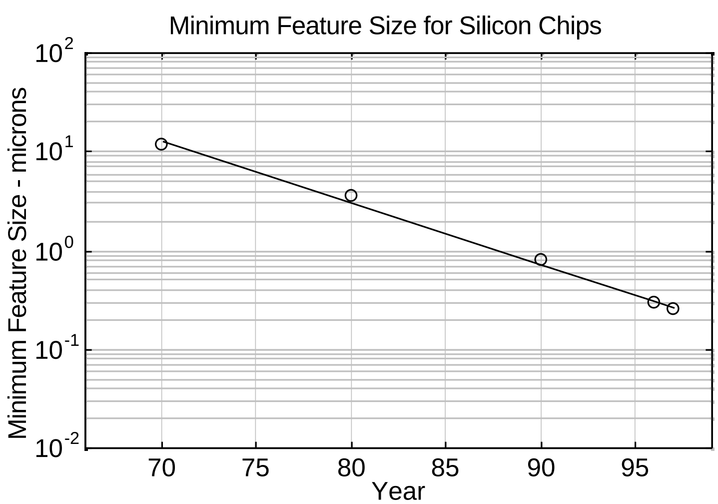


Figure 3. Minimum feature size for silicon chips.

Thus new technologies using photolithography with much shorter wavelengths or, more likely, completely new technologies not involving the interplay between light and photoreactive polymer resists, will be required. The new technologies may involve very-difficult-to-focus x-ray or rather slow electron beam processing (used by NEC in development of the experimental 4 Gbit DRAM chip mentioned earlier).

IBM researchers have reported creation of microstructures on silicon as small as 30 nanometers, and many university and corporate researchers worldwide are working on development of the ultimate smallest silicon component, the single-electron transistor, for which the minimum feature size is about 7 nanometers. Thus, for transistor-based micro-electronic silicon chips there *will* be an ultimate maximum transistor density and minimum feature size, whatever chip fabrication technology supplants photolithography. If the trend toward smaller feature size illustrated in Figure 3 were to continue unabated (improbable), that ultimate limit, two orders of magnitude smaller than 0.1 micron, would be reached sometime around 2025.

From the numbers cited in the previous paragraphs, it appears likely that the rapid increases in transistor density (hence computer performance) we have seen in past decades will continue for at least one more decade. Whether the pace continues for the decade after that will depend as much on the development of cost-effective manufacturing techniques as on theoretical possibilities. The sheer cost of a new “fab” (chip fabrication plant) may, in fact, determine when Moore's Law (transistor density doubles every eighteen months), first postulated in the mid-1960’s by a founder of Intel, finally breaks down. The capital investment in a typical fab has climbed from about $1 million in 1970 to about $1 billion in 1994 to about $2.5 billion for a new Texas Instrument 0.25 micron fab scheduled to become operational in 1997.

Given that gross revenues for the largest chip maker, Intel, will be approximately $25 billion in 1996 (and growing at a compounded rate of about 35% per year) it seems doubtful that more than a very few companies worldwide will have the resources to create fabs based on entirely new technologies that may well cost $10 billion each by 2005 or so when the current photolithographic process will have run its course. $10 billion is not small change for any company; it is about 10% of the current *combined* market capitalization of the Big Three US automakers.

Parallel Processing

This is not to say that computational power of typical, affordable computers will at some point fail to grow at the exponential rate we are accustomed to. What cannot be accomplished with speedier individual processors will be made possible by processing in parallel on more than one.

The supercomputing and parallel processing paradigm is currently going through perilous times, as several once-prominent companies have either gone bankrupt or been taken over by larger ones whose major revenues come from more conventional computer and/or workstation sales. One current trend that seems certain to continue involves use of off-the-shelf mass-produced (typically RISC) processors, rather than extremely fast but very expensive custom-designed processors, such as have traditionally been used in the fastest supercomputers with pipelined vector architectures. At least one experimental parallel machine with over 9000 processors (from Intel, using Pentium II CISC processors) has already performed useful calculations at speeds exceeding 1 Teraflop (trillions of floating-point operations per second), almost three orders of magnitude faster than the fastest current custom-built supercomputer processor made by Fujitsu. By 2001 a 10-teraflop machine (to be built by IBM for the Energy Department) will be in operation at the Los Alamos or Livermore National Laboratories.

Currently, two general architectures predominate, one called SYM (symmetric multiprocessing), involving a shared memory accessible (either directly or indirectly) by all processors, and the other called MIMD (multiple instruction, multiple data) involving networked processors, each having its own “private” memory, inaccessible to the other processors.

Each of the architectures has its strengths and weaknesses. Programming of SYM machines is simpler than for MIMD machines (though explicit synchronization is required to avoid data access “races” by contending processors). For machines with a small number of processors (for example, just a few for desktop machines), the SYM architecture is likely to dominate. Unfortunately, as the number of processors grows, the bus structures for the shared memory SYM machines can become extremely complicated, so scaleup to massive parallelism (beyond say a few hundred processing nodes) is difficult technically and very expensive.

On the other hand, the networked individual processor MIMD model typically requires message-passing software such as PVM (Parallel Virtual Machine) or MPI (Message Passing Interface) to explicitly request transfer of information from one processor’s memory to the memory of another processor that needs it. This complicates software development. The individual processors on these parallel machines behave like individual workstations with each node, normally running its own copy of the (Unix) operating system, attached to a local area network (albeit a very, very fast one, called a *switch*). Because of the architecture, MIMD machines are inherently scalable to quite large numbers (many thousands) of processors.

Parallel programs for tightly-switched MIMD machines can often be run as easily (though not as quickly) on networks of workstations. My guess is that this model will be the predominant one for engineering computing by 2001. Software to ease the programming problem is coming to market, and there will be a vast resource of unused compute cycles on very high performance networked workstations already in place in most engineering-oriented businesses (and universities), just waiting to be exploited for solution of computationally complex problems.

Communications

Without doubt, communications is the “computing” area experiencing the greatest acceleration in growth and greatest decrease in price/performance ratio. Daniel Atkins, Dean of the School of Information and Library Sciences and Professor of Computer Engineering at Michigan, estimates (personal communication) that the price/performance ratio for communication bandwidth is currently decreasing at a rate ten times that for computing hardware.

Tables 1 and 2 show the astounding impact of the capacity of storage media and network bandwidth on the storage and transmission of typical documents (here for uncompressed text only). Note also that the recently released single-side/single-layer DVD (Digital Versatile Disk) has about eight times (4.7 GBytes) the capacity of the conventional CD ROM listed in the table. If two layers per side (read by adjusting the focus of the laser) and both sides are used, then a single DVD, physically the size of a CD, can store a total of 18.8 GBytes, equivalent in capacity to 32 current CD ROMs. So all the text (but not the graphics!) in all the documents in the Library of Congress could be stored in fewer than 1000 such DVDs. (Don’t expect to see this anytime soon! The Library of Congress is currently creating a digital library by scanning at high-resolution about 1 million new and recent documents per year; the library will be available to K12 and university libraries as an on-line resource. Digitizing all 20 million documents in the Library would be a massive and expensive undertaking, and is unlikely to be funded.)

The fastest local area network data-transmission rates, about 5 Mbps (millions of bits per second) in 1980, will certainly be greater than 1 Gbps by 2001 (1 Gbps Ethernet equipment will be available from manufacturers sometime in 1997). Milti-gigabit rates for high-performance switched networks, such as those used in massively parallel MIMD machines, will also be common by 2001.

Table 1: Sizes of Typical Stored Documents (Lucky)

Document	Bytes	Floppy Disks	CD ROMs
Page	2,400	0	1
Report	72,000	0	1
Book	720,000	1	1
Dictionary	60,000,000	43	1
Encyclopedia	130,000,000	93	1
Local Library	70,000,000,000	50,000	108
College Library	700,000,000,000	500,000	700
Library of Congress	18,000,000,000,000	12,900,000	26,000

Table 2: Transmission Times for Typical Documents (Lucky)

Document	Modem 28,000 bps	T1 (1.5Mbps)	Fiber Optic (1.7 Gbps)
Page	0.68 sec	0.013 sec	0.0000113 sec
Report	20.5 sec	0.38 sec	0.000339 sec
Book	3.42 min	3.84 sec	0.0034 sec
Dictionary	4.76 hr	5.3 min	0.28 sec
Encyclopedia	10.32 hr	11.6 hr	0.61 sec
Local Library	232 days	4.32 days	5.49 min
College Library	6.34 yr	43.2 days	0.92 hr
Library of Congress	163 yr	3.04 years	23.5 hr

In late 1996, fast backbone Internet lines operate at about 45 Mbps. By the end of 1997, the facilities of a yet faster Internet, called vBNS (very high speed backbone network service) or Internet II, will connect about 100 research Universities and the national supercomputing sites with optical backbone connections operating at 155 Mbps. No doubt Internet II will, in turn, be replaced by Internet III, having a substantially greater bandwidth. Gigabit Internet backbone service will almost certainly be available for at least some users by 2001.

Most current modems attached to commercial cable television networks support Internet transmissions at T1 rates (1.5 Mbps), some 50 times typical telephone modem rates (28.8 kbps). Potentially, however, broadband cable modems with optical cable lines are capable of very much higher data rates, in the 10 to 40 Mbps range, at least when downloading (transfers from the Net to local PC); uploading (PC to Net) is normally slower, but still several times faster than for current telephone modem communication. Unfortunately, only about 10% of current commercial cable systems support two-way communication at all (so that PC to Net transmissions require a separate telephone modem), a situation that will probably be remedied by 2001 as companies upgrade their equipment and replace copper lines with optical ones.

Wireless services are now pervasive, and relatively inexpensive. Wireless local area networks are proliferating, and represent a cost-effective alternative to copper or optical cabling as a way of "wiring" a building (though the data rates cannot compete with those for high-bandwidth optical fiber). Several different sets of globe-girdling LEO (low-earth-orbit) satellite systems are about to be put into place by consortiums of computing and communication companies. They will provide high speed wireless services from virtually any place on the earth's surface. For example, 28 Mbps wireless Internet connections are planned for the $9 billion Microsoft/McCaw/Boeing Teldesic system of 288 satellites, scheduled to be fully operational in 2001.

The Web Changes Everything

Local (LAN) and wide area (WAN) networks have been with us for about twenty five years, starting with the Ethernet LAN, developed at XEROX PARC in the early 1970s, and the wide-area ARPANet, for which the first machine to machine transmission (from the University of Southern California to the University of California at Berkeley) took place in September 1969. Prior to the development of these technologies, most remote computing was performed at dumb terminals connected by telephone modem to mainframes operating in time-sharing mode.

Local area networks (LANs) made possible the high-speed sharing of resources such as mass storage units and printers. With the development of Unix in the late 1960s and early 1970s, remote computational resources on the network could also be tapped by multiple users directly from their own networked machines.

ARPANet allowed for remote messaging (EMail) and file transfer, and the sharing of ideas, data, research results and computational resources among users of machines that were widely separated geographically. A key breakthrough came with the adoption of the Internet transmission protocol (TCP/IP) and Internet domain addressing scheme in 1974. TCP/IP created a universally recognized standard for transmission of information "packets" over the network, and the addressing standard supported creation of world-wide directories, allowing unique identification of every networked machine and the speedy delivery of information packets to their intended target machines.

With support from the US Defense Department, ARPANet grew at a steady but unspectacular pace during the 1970s from 24 sites in 1971 to about 200 in 1981. In 1986 ARPANet was replaced by a less "military," more academic, network called NSFNet. One of the principal functions of NSFNet was to provide high bandwidth access between University campuses and five National Supercomputing sites (reduced to two in 1996). NSFNet was in turn replaced by the loosely (some believe chaotically) managed, rather amorphous Internet (a network of networks) in the late 1980s. As of late 1996, the world-wide Internet ties together more than 100,000 individual networks with more than 50 million attached (either directly or through Internet service providers) individual machines.

The incredible recent growth in Internet infrastructure and use can be attributed in large part to the development of the World Wide Web (*www* or simply *the Web*), which allows for easy access to *hyperlinked* documents stored on any accessible machine located anywhere on the Internet. Hypertext, which permits the nonlinear linking (essentially without restriction) of one piece of information with another (presumably related) one, was first suggested by Vannevar Bush (see earlier) in 1945, and was promoted by researchers at XEROX PARC in the early 1980's as a way of referencing and retrieving related information.

Tim Berners-Lee, an English physicist working at CERN in Zurich, is credited with developing three key Web concepts in the late 1980s and early 1990s:

A standard language for encoding hypertext documents.

A standard Internet protocol for linking and transmitting hypertext documents.

An addressing system for locating documents.

The language HTML (hypertext markup language), protocol HTTP (hypertext transfer protocol), and addressing system URL (universal resource locator) form the underpinnings of the current Web. One of the key decisions made by Berners-Lee was that a central directory (which would allow for deleting and updating links as hyperlinked documents were removed or modified) was infeasible for a "World-Wide" information web, i.e., that "dangling" hyperlinks to a removed document would simply have to be tolerated for the greater good of allowing independent actions by individual Web document owners.

In 1990, Berners-Lee developed a browser/editor at CERN for creating, accessing and displaying hypertext documents (principally research papers and data at CERN) using his HTML, HTTP, and URL concepts. However, it was not until 1993 when the Mosaic browser was created at NSCA (University of Illinois), that the potential of the Web became apparent (at least to some). With the formation of Netscape, Inc. and the release of the Netscape browser in 1994, the Web "took off".

The principal resources that can be hyperlinked on the web go far beyond mere text, indeed can be almost anything (text, graphics, sound, animation, video, virtual reality images, signals from an instrument on a remote experiment, software, ...); essentially any information that can be digitized can, or soon will be, Web-linkable.

It is, I think, fair to say that the Web changes everything. If, as McLuhan suggested in 1967, the medium is the message, then here the message is the Web. Some (myself included) think the Web may be as revolutionary an invention affecting the way we communicate and access and disseminate information as was the printing press.

The Web is the first truly new medium since television; it is, in fact, a multi-medium because the range of resources it can access potentially includes essentially all of the other mass media (newspapers, movies, radio, television). But in addition to providing a vehicle for "push" technology or "webcasting," in which the Net delivers information to the user (much as broadcasters do), the Web (1) allows an individual user to *interact* with resources and other users on the Web, and (2) allows an individual user to *create* resources, in essence to become a "publisher," without formal approval by an oversight authority. The Web can be an extraordinarily liberating medium for individual creativity (much that is worthless gets created in the process as well). The Web (or whatever supplants it) is clearly a multi-medium destined to have enormous impact on information dissemination, education, and commerce.

The Web's growth during the past three years is simply phenomenal. Virtually every corporation, academic institution, government agency, and uncounted individuals now have a presence on the Web, at least in the form of a hyperlinked home page.

Commercial Web activity is growing apace. It is hard to believe that the first commercial advertisement on the Web (for a lawyer's services) (1) raised a furor among Web users as a violation of Web etiquette, and (2) happened as recently as April 19, 1994. Contrast this with an estimate by Forrester Research that commercial Web transactions will exceed $10 billion in 1999, with computer hardware and software sales comprising a large piece of the commercial pie.

The recent flurry of multi-billion dollar buyouts and takeovers involving television, telephone, wireless, cable, computing and on-line Net-access companies attests to the fluidity of the situation and to the uncertainty about which technologies or combinations of them will eventually win in the "interactive" educational, entertainment, and commercial marketplace. My guess is that by 2001 commercial and educational interactivity will be centered on the Web and computer (with commercial cable systems providing Net connectivity for a substantial fraction of home users), rather than on interactive cable and the television set. News and entertainment currently delivered by mass media will stay in the domains of newspapers, radio, movies, and television, but the Web will play a role in these areas too (on-line magazines, webcast stock market reports and breaking news, etc.).

Perhaps the Web's greatest impact has been on the nature of "computing" itself. The center of gravity for computing activity is shifting perceptibly from individual computers and workstations to the network. Major corporations such as IBM and Microsoft have reoriented their missions to focus on delivery of "Net-centric" services and "Net-aware" application software. The distinction between what's done locally and what's done remotely will blur substantially in the coming years. Many corporations have already taken advantage of the net-centric Web model by creating internal internets called *intranets*, mini-Internets that use standard Web software such as browsers for accessing and updating corporate data and information; firewalls (software to isolate the internal intranet from the Internet) protect corporate information from the outside world.

Because the Web is so new and has grown so rapidly, it has many rough edges and problems. Service can be slow; breakdowns do occur (and will surely continue to occur). However, the Net's distributed nature and redundancy of communication paths virtually insures that only parts of it will be affected by a particular failure; a catastrophic Net breakdown comparable to a nation-wide power outage seems unlikely. On balance, the commercial carriers have done a remarkable job in installing new lines and equipment in response to rising demand, and will undoubtedly continue to do so, as a wholly new optical fiber and wireless communication infrastructure takes shape over the next decade.

Two issues that need to be addressed before the Web can reach its full potential in the commercial arena are: (1) security of Web-based financial transactions, and (2) copyright protection for Web-accessible intellectual property. The problems in these areas are challenging both technically and legally, and too involved to discuss here (and I don't know much about them!).

Substantial work has been done on financial security issues, mostly involving some form of encryption, and the Web is already being used fairly heavily for on-line sales and financial transactions, with apparently little fraud or error (but the occasional horror story shows that problems exist). US copyright laws are under active discussion in the Congress, and an International Copyright Convention of 160 nations, meeting during 1996 and 1997, will attempt to reach global agreement on the handling of intellectual property, particularly computer-based intellectual property. Real copyright protection is more likely to come from the bottom up (in the form of technical safeguards on the Web) than from the top down (international treaties or US copyright law). Because these issues are so important to the future of the Web and to the use of Web-based information for commerce and education, I believe that some reasonable and effective solutions for current security and copyright problems are likely to be in place by 2001.

Software

The most important software for engineering students, faculty, and professionals can be broadly classified by general function: (1) system software, (2) network services, (3) programming language translators/compilers, (4) general productivity tools, (5) problem, task, or discipline-oriented applications, and (6) multi-media instructional aids.

System software includes the base operating system for the computer and a myriad of programs for providing communication and access to system resources. The first operating system, for controlling the processing of batches of programs on punched cards on the IBM 704, was released in 1957. Subsequent systems, for time-shared access to mainframes, appeared in the mid-1960s. With each new class of hardware (minicomputers, personal computers, workstations, etc.), new and usually more sophisticated operating systems appeared and then slowly evolved over the years.

Currently, the most important operating systems are Unix, used on engineering workstations with RISC processors, Windows95/DOS and Windows NT for personal computers with Intel and compatible processors, and the Macintosh OS for Macintosh and clones with Power PC processors. All now have graphical user interfaces that are descendants of windowed interfaces developed at XEROX PARC in the early 1970s and popularized with release of the Macintosh in 1984; the interfaces appear remarkably alike to the user, making switching from one machine to another much less onerous than in earlier times (but still not without pain!).

New features such as support for multiple users (Unix), preemptive multi-tasking (time-sharing of the local processor among several running programs), threads (parallel minitasks within a single application), and network services (e.g., remote file transfer, electronic mail, Internet and Web access) have over the years been incorporated into or made available to operating systems.

Future versions of the predominant operating systems will almost certainly be much more "network-aware" than current ones, i.e., it is likely that the user interface (probably with a three-dimensional appearance) will eventually make little distinction between what is local to the user's workstation and what is on the network or Web.

The desktop metaphor with its emphasis on files and folders has been dominant since the introduction of the Macintosh in 1984, but is giving way to new metaphors, in particular that of the compound document as a container for objects - textual, graphical, sound, video, computational. Group interfaces for conferencing and for working collaboratively over the network are under development, and likely to be very important in both the academic and industrial workplace by 2001. Virtual reality will almost certainly play a role as a 3-dimensional imaging tool for navigating in the net-centered operating systems of the future. New multi-sensory tools involving gesture, eye and body motion, voice, smell (maybe not!) will eventually supplement the keyboard and mouse for interacting with those future operating systems.

Stephanopolous and Han (see p. 239) have described programming language developments in lucid detail, so I won't elaboratye on their observations here, except to note that there are strong trends toward development of modular, structured, and more easily maintained and reusable object-oriented programs (the latter allow for hierarchical decomposition, and encapsulate both data structure and algorithm). My guess is that by 2001 most chemical engineering students will be trained to use high-level and visually-oriented computational and "programming" tools rather than traditional procedure-oriented languages such as FORTRAN and C.

In general, software improvements come much more slowly than those for hardware described earlier. This results from the fact that much code is still "handcrafted," that many popular applications were originally written years ago with unstructured code, that subsequent "improvements" have been made in ad hoc fashion, and that programs are often quite large (many are enormous), hence difficult to validate.

Nevertheless, there is hope from a new computing discipline, software engineering, from object-oriented programming technology, from the trend toward open systems, cross-platform (different kinds of computers) compatibility, emerging international standards for communications and hardware interfacing, and, in some cases, cooperation among software developers and hardware manufacturers.

One of the most exciting recent software developments is the emergence of Sun Microsystems' Java, an object-oriented language for creating programs that reside on network servers. When a networked user requests a service or a calculation or a display provided by a Java program (small ones are called applets), the Java code is downloaded to the user's workstation from the server, and either immediately interpreted locally by a *Java virtual machine* (JVM) translator or compiled into machine code for the workstation and executed. JVMs are available for essentially all personal computers and workstations and are being incorporated into Web browsers such as Netscape and Microsoft Explorer and other application programs.

This means that a Java program automatically has cross-platform compatibility (Nirvana for a programmer), since it can be run without modification on any computer, such as a Unix workstation, Macintosh, or "Wintel" (Windows operating system and Intel processor) machine with a JVM or Java-compliant browser. The user need not store the program locally, and the Java programmer can change the program without concern for the machine it will eventually be run on. Java, or some successor to it, is central to the notion of Net-centric computing.

Sun and a few other hardware/software vendors view Java as the tool for creating network-centered operating systems to replace conventional workstation operating systems such as Windows and the Macintosh OS, treating individual machines as network computers. My guess is that this will not happen, and that conventional operating systems will instead become much more Java-compliant by incorporating JVMs and Java compilers as core components.

Many other new software developments are also Web oriented, especially for creating and improving search engines for locating and cataloging URLs of interest on the Web, and for creating intelligent Web agents (small programs that move about the Web searching data bases and filtering information to carry out specific tasks of interest to the user). Current Web search engines are quite primitive, and identify URLs of interest based on text matching only. Engines available in 2001 will likely allow for searching of text in context and searching of non-textual information, in particular, images (e.g., find pictures containing sunsets) and sounds (e.g., find soundbites with references to global warming).

Implications for Chemical Engineering Education

How do (and will) all these intense (and accelerating) computing activities affect academia in general and engineering education in particular? In many respects, the impact of computing on education and academic life has paralleled that in the world outside the academy. Substantial basic research that feeds the computer revolution is performed by academics and their students. The University of the present looks quite different from the University of even a decade ago. Virtually every desk supports a networked desktop computer, the University library is "on-line," and every dorm room is (or soon will be) connected to the rest of the electronic world. The computer has brought with it systemic changes in the ways the University conducts its business and research and interacts with its students, graduates, faculty, and staff.

The impact of the computer *in* the classroom has, to date, been much less dramatic than in other areas of the academy. An 1896 still photo of an engineering classroom, professor lecturing with chalk in hand, would look remarkably similar to most engineering classrooms in 1996. Will that paradigm last for yet another century? Not likely.

Despite its apparent lack of impact to date in most classrooms, the computer has certainly affected what we teach and how students learn, as is evident from the many earlier papers in this monograph. Most chemical process design [Biegler, Seader and Seider (p. 153), Grossmann (p. 171), Grossmann and Morari (p. 185)] and many control (Arkun and Garcia, p. 193), and separations processes (Taylor, p. 139) courses have already been transformed into computationally centered ones. Most undergraduate laboratories have also undergone major upgrading, and the computer is now an integral part of experimental systems, both for data acquisition and data processing, as described by Mellichamp and Joseph (p. 203).

Interactive multi-media instructional tools, such as those described by Fogler and Montgomery (p. 57) and Fogler (p. 103), allow faculty to create remedial and supplemental tools for self-paced learning of course material that are particularly effective for students whose learning styles differ from the linear, analytical learning and teaching styles of most faculty. Numerical mathematical tools, described by Shacham, Cutlip, and Brauner (p. 73), allow students to solve nonlinear model equations and to carry out simulations that could not easily have been included in core engineering science coursework in thermodynamics (p. 85), transport processes (Finlayson and Hrymak, p. 125), and reaction engineering (Fogler, 103), as recently as a few years ago.

Nevertheless, the overall impact of the computer in our undergraduate curricula, particularly in our core chemical engineering science courses, has been less than might have been expected, given the computing resources now available on most engineering campuses. As pointed out by Kantor and Edgar (p. 9), most of our standard textbooks do not yet have a significant computer-orientation. I foresee the standard textbooks of the next century as much different from those of the past. The future text will not be structured as the linear sequence of static information found in our current texts, but will contain hyperlinked navigational aids, animation and sound, tools for manipulating data, and programs for carrying out simulations with user-supplied inputs. By definition, they will require the computer for their use, and may even be completely Web based, with small charges assessed for each access. (No doubt students will still want to print many screen images as they appear, so even these “electronic” texts are likely be accompanied by hard copy materials).

Most classrooms are not yet equipped with ready-to-use networked computing and projection facilities needed for doing good in-class demonstrations. Such equipment represents a significant investment by the university, but it will be essential for engineering classroom instruction in the next decade. Classroom visualization (Hrymak and Monger, p. 253) of the unfolding dynamic solution of a fluid mechanics problem is worth much more than a thousand faculty words.

Creation of good computer-oriented instructional materials and stimulating in-class demonstrations (even with the best computing and display equipment in place) is challenging, time-consuming, and expensive. Unfortunately, such efforts by faculty often receive little recognition by department chairs and deans, particularly at research universities, so we may continue to see fairly slow progress in fully integrating computing work into our core engineering science courses.

On the other hand, the Web could revolutionize the way we manage course-related activities. By 2001, virtually every course will have a home page on a Web site, with links to class schedules, problem assignments and solutions, interactive messaging, and student records. Driven by faculty interest and commitment, some courses will be strongly Web-centered, with facilities for student collaboration and group interaction, in-class note taking (using laptops with wireless communication?), interactive multi-media tools that integrate materials from local machines, CD ROM and the network, on-line examinations, and access to a wide array of data base resources and numerical and discipline-specific software; classical lecture presentations in these courses will diminish in importance. Some departments may have full-time Webmasters whose principal duties involve assisting faculty in bringing the curriculum to the Web.

The Virtual University?

Viewed more broadly, the new computing technologies, and particularly the Web, promise to transform the way Universities keep in touch with their alumni and deliver continuing education to professionals. As the bandwidth of Internet trunk lines rises dramatically in the next decade, videoconferencing, on-line interaction and collaboration, and Web access to digital data bases and libraries will make cost-effective delivery of distance learning a reality.

Some Internet-based experimental distance learning experiments are already underway. One, a joint venture of the University of Michigan, the State of Michigan and the auto industry called the "Virtual Automotive College," is being directed by James Duderstadt, a former Dean of Engineering and now President Emeritus of the University. The virtual college will deliver its first all-electronic courses to engineers in the automobile industry over the Internet during the Winter term of 1997.

In theory, a "virtual university" could be created using the new computing and communication tools and instructional technology with the Internet as its infrastructure. The driving force behind such a university would be delivery of instruction to large numbers of students and professionals in their homes or workplaces at much lower cost than with traditional campus-based courses. However, unless students have access to substantial interaction, group collaboration, and the opportunity to form learning communities, I'm skeptical of the near-term success of such a university, at least for young (18 to 24 year old) students. A college education involves much more than passive learning in near isolation. As suggested by Brown and Duguid, social experience, groups joined, scholars worked with, friendships made, prestige and marketability of degrees earned, and a sense of place play powerful roles in the College experience. It seems unlikely that a virtual university will ever be viewed with nostalgia as *alma mater*.

Summary

I have attempted to give an overview of past developments and current trends in digital computing and communications (in particular of networks, the Internet, and the Web), and to make some predictions about what the computing world will look like half a decade hence, in 2001. Many of the facts and figures are unattributed; for the most part, they come from extensive notes taken and articles (from newspapers, trade magazines, technical journals) clipped over many, many years.

The conjectures about the future are mostly my own; fortunately I can't be proved wrong until 2001, at which point the whole exercise can be done again!

References

Brown, J.S., and P. Duguid (1995). Universities in the Digital Age. Position paper, XEROX PARC, Palo Alto.

Hennesey, J.L., and D.A. Patterson (1995). *Computer Architecture: A Quantitative Approach*. Morgan Kaufmann, San Francisco.

Stix, G. (1995). Toward "Point One." *Scientific American*, (2), 90-95.

Lucky, J. (1989). *Silicon Dreams*. St. Martins Press.

Individual inquiries should be addressed to:

CACHE Corporation
P. O. Box 7939
Austin, Texas 78713-7939
(512) 471-4933
FAX: (512) 295-4498
cache@uts.cc.utexas.edu

http://www.cache.org

CACHE NEWS

The CACHE News is published twice a year and reports news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by Christine Bailor with contributions from a number of CACHE members and representatives.

CHEMICAL ENGINEERING EDUCATION AND THE THREE C's: COMPUTING, COMMUNICATION, AND COLLABORATION

Thomas F. Edgar

Department of Chemical Engineering
University of Texas
Austin, TX 78712
edgar@mail.utexas.edu

Key words: information technology, computing, distance education, simulation, numerical analysis

Presented at the 2000 Annual Meeting, Los Angeles, CA, November 12-17

Session: Chemical Engineering Issues of the New Millenium: Beyond Vision 2020

ABSTRACT

As we enter the 21st century, it is clear that chemical engineering education will be profoundly influenced by the Information Age. The three R's that were the basis for education in the beginning of the 20th century will be replaced by the three C's arising out of information technology: computing, communication, and collaboration. Within chemical engineering education computing is well-established in every course in the curriculum but there is considerable potential for growth and enhancement. The present trends toward greater user interaction and visualization will continue, and tools like simulation will grow in importance, lessening the typical user's need to know about the underlying numerics. The use of digital communication will automate laboratory experiences and make them more productive. Communication tools such as digital libraries and Internet 2 will also greatly enhance the student and faculty experiences. Collaboration will become more palpable in changing current modes of instruction and research. The use of multimedia will transform both classrooms and content presentation and can enhance the learning experience of all students.

Introduction

The transformation from the Industrial Age to the Information Age is having a profound impact on both industry and academia. Universities have moved to networked environments that permit faculty, staff, and students to have access to the World Wide Web anytime and anywhere. Many faculty are beginning to use information technology (IT) to enhance the collaborative component of education, with an increased focus on the learning process. They will share courses over the Internet, access digital libraries, write electronic books, and perhaps even form a virtual chemical engineering department using digital shared content from multiple departments. We have already seen the formation of networks of faculty, who share research ideas and data over the Internet on a daily or hourly basis (a virtual collaboratory).

The expectations and needs of incoming students for digital facilities and curricula are being shaped by a world of pervasive microprocessors and telecommunications in their lives. They are equally comfortable talking on a cell phone or using asynchronous communication by chat or e-mail. Their entertainment is found on the world-wide web, e.g., music is provided by sharing of computer files (cf. Napster). The new digital generation is not intimidated by computers, demands interaction, views learning as a plug and play experience, won't read a manual but learns through experimentation, expects well-designed user interfaces, and may not learn best through the linear seriatim process. Given the current students in universities and the expanding capabilities of informative technology, the role of the computer in engineering is expanding from simply computing to include communication and collaboration (the three C's).

2.0 Computing in Chemical Engineering Education

The capacity of computing hardware has improved by orders or magnitude over the past forty years evolving from mainframes to today's multifunctional personal computer/workstation. These striking developments have occurred while cycle costs have been greatly reduced, and the computer has become a ubiquitous tool for increased productivity in engineering practice. Prior to the mid-1980s, the lack of professional software and inexpensive computing equipment limited computing experiences for undergraduate engineers, but no such constraints exist today. Historically the use of computing in the curriculum has focused mainly on a single course: numerical analysis. Starting in the 1990s, commercial simulators such as ASPEN, PRO-II, CHEMCAD, and HYSIM were widely adopted in universities via educational discounts, aided by user-friendly interfaces (front-ends) and PC-based software packages. The use of computer-aided simulation in the capstone senior design course can certainly be characterized as a major success story in the education of chemical engineers. However, the ubiquitous nature of PCs on university campuses has not yet caused a quantum change in the way computing is taught or applied in the typical chemical engineering department, nor is the use of computing pervasive throughout the curriculum in a typical department.

In courses such as thermodynamics, transport phenomena, unit operations, separations, and reactor design, there is still only a modest level of computation at many universities. Certainly in the thermodynamics and separations area, there is a lot to be gained by introducing simulation packages and molecular modeling subroutines. Sandler's latest edition on thermodynamics has a set of computer disks including equations of state and connections to TK Solver. Reactor design is a particularly interesting case, in that powerful numerical solution methods for reactor design, ordinary and partial differential equations, and parameter estimation for these systems have not been utilized in most textbook presentations. However, the most recent edition of the leading textbook in reactor design by Scott Fogler has introduced interactive computer exercises for demonstration of important concepts, and utilizes Polymath for reactor simulation. Another reactor textbook forthcoming by John Ekerdt and Jim Rawlings makes extensive use of numerical analysis via Octave. Both Polymath (www.cache.org) and Octave (www.che.wisc.edu/octave) were developed by chemical engineering educators but have applicability outside of this field.

Some courses in chemical engineering, such as process control and optimization, are computer-intensive by their very nature, and there are quite a few professional PC-based software packages that are available for student use, sometimes via the world wide web. Today packages such as GAMS offer easy-to-use interfaces to combine algebraic modeling procedures with optimization to solve almost any linear or nonlinear programming problem (including integer variables) of reasonable size. Many of the major libraries of mathematical software include individual callable routines for most variations of numerical analysis and optimization. The NAG Fortran Library (available as a toolbox of MATLAB) contains routines which perform such tasks as equation solving, unconstrained optimization, and various linear algebra operations.

In the 1980's a major move away from FORTRAN and C optimization began as optimizers, first LP solvers and then NLP solvers were interfaced to spreadsheet systems for desktop computers. The spreadsheet has become a popular user interface for entering and manipulating numeric data. Spreadsheet vendors are increasingly incorporating analytic tools accessible from the spreadsheet interface that permit access to external databases. Examples include statistical packages, optimizers, and equation solvers.

Microsoft Excel incorporates the routine, SOLVER, which operates on the values and formulas of a spreadsheet model. Current versions (4.0 and later) include an LP solver and mixed integer programming (MIP) capability for both linear and nonlinear problems. The user specifies a set of cell addresses to be independently adjusted (the decision variables), a set of formula cells whose values are to be constrained (the constraints), and a formula cell designated as the optimization objective. The solver uses the spreadsheet interpreter to evaluate the constraint and objective functions, and differences those computations to generate derivatives. The NLP solution engine for the Excel solver is GRG2.

Process control courses have adopted a defacto standard of MATLAB for dynamic simulation and controller design (www.mathworks.com). MATLAB is augmented with a large number of specialized toolboxes, many of which originated from academic software developed by faculty and graduate students (e.g., model predictive control toolbox). Graphical presentation of results makes these packages useful for iterative design and analysis, and graphical user interfaces such as SIMULINK make solving closed-loop analysis problems much easier than using either transfer function or state space equation formats. So far the only textbook with extensive use of MATLAB-based homework problems is by Tom Marlin, although it is planned for the next edition of Seborg, Edgar, and Mellichamp.

What about the needed computing skills in the undergraduate curriculum in the future? The focus should be on what kinds of experiences and computer-enhanced problem-solving abilities chemical engineers must have when they graduate. B.S. Ch.E graduates should:

1. Know how to use a modern technical library to search for information located in electronic databases, and how to access electronic information services through the World Wide Web.

2. Understand the implementation of elementary algorithms for the numerical solution of engineering problems. These algorithms should include algebraic and differential equation solving, linear algebra, and optimization.

3. Be able to solve more sophisticated engineering problems using appropriate applications software. The types of problems include material and energy balances, optimization problems with constraints, and statistical data analysis.

4. Be familiar with software for computer-aided process design and analysis.

5. Have experience with computer-based instrumentation, process control, data collection, and analysis.

How should this material be taught? Courses should teach how to implement elementary algorithms for problem-solving. The most useful tools are numerically oriented and allow students to explore the use of different algorithms, problem formulation, and means to visualize the results. Note that programming language expertise is not included in the above list. There are several excellent higher-level language alternatives for numerical analysis as a required course, including MATLAB, Mathematica, and Maple. These tools allow one to script solution algorithms very efficiently, and include excellent visualization and problem-solving toolboxes. Using such metacomputing tools allows omitting FORTRAN as a required course from the undergraduate curriculum in favor of these alternatives.

Ideally, students would enhance their computer-based problem-solving skills continually as they pass through the standard curriculum. Thermodynamics, fluid mechanics, and heat and mass transfer allow many opportunities for students to solve problems involving algebraic equations, integration, data regression, and challenges in visualizing solutions. Reaction engineering process design and process control and design courses offer opportunities for dynamic simulation of realistic models.

3.0 Communications

The digital science and information revolution is rapidly transforming the ways faculty and students collaborate, solve problems, and disseminate knowledge. The integration of computers, telecommunications, audio, video, multimedia, and other digital technologies creates a worldwide information environment that can be accessed easily from the laboratory, office, field, and home. While it is difficult to perform experimental research at a distance, sharing of expensive specialized equipment through virtual connections will become more common in the future. Faculty in the future will rely more heavily on computational and visualization tools, with relatively less investment in equipment and laboratory facilities. Experimentation is relatively more expensive to perform with today’s stringent safety requirements. Most faculty will need to stay up to date in some aspects of IT in order to carry out cutting-edge research, which may impact the types of faculty hired by chemical engineering departments.

Most U.S. universities are now members of Internet 2, which provides high bandwidth capabilities (over 100 times as fast as today's commodity Internet) for faculty communication and distance education. This includes, for example, digital libraries with audio and video content, collaboration and immersion environments, remote monitoring of experiments, and data-intensive applications (see www.internet2.edu).

4.0 Collaboration

Collaborative tools now allow researchers throughout the world to share results regularly, on a daily or even hourly basis via informal collaboratories. This of course can be expanded to educational materials, where faculty can share software and educational content over the world wide web, thus mitigating the "not invented here" mentality that is common in most universities. One attempt to foster such cooperation in chemical engineering education is the new web site www. cache.org, sponsored by the CACHE Corporation.

Electronic publishing and the gradual replacement of paper-based modes for carrying out the business of higher education will certainly impact chemical engineering education in the future. We have seen the first wave of construction of digital libraries; both the American Chemical Society and Elsevier are being fairly aggressive in moving toward complete digitization of scientific and engineering journals, while AIChE has proceeded more cautiously. Clearly both faculty and students find having access to the text of journal articles and other digital content on one's desktop to be a tremendous productivity tool.

Electronic books may eventually replace part of the traditional book publishing market. The high cost of textbooks and the collective weight of five books in a backpack are certainly incentives for students to use electronic media in the future. Computer companies are developing devices that feel like a book but permit downloading of material from the web.

Significant progress in changing the paradigm of textbook publishing may occur over the next five to ten years, where the contents of a book would be entirely on-line. This would be advantageous for incorporating interactive exercises based on simulation in an integrated way, converting the traditional textbook into courseware that is much more comprehensive than the hard copy versions used today. This would allow faculty to selectively incorporate parts of books into their courses. Perhaps the best example of an electronic book combined with a distance education course in chemical engineering has been developed by Scott Fogler (see http://www.umich.edu/~cre/ .   Another electronic textbook under development that bears watching is on molecular modeling (see http://flory.utk.edu).

Collaborative Approaches to Teaching and Learning

Collaborative learning environments can be active agents that interact with students, expand the information horizons of students, and enable effective interactions across both time and distance. Use of such systems in teaching and learning is growing rapidly. In such environments a computer presents and combines text, graphics, audio and video (multimedia), with links and tools that let the user navigate, interact, create and communicate. This technology can interact with students in new ways, e.g., to give students experiences through simulations of logical and physical systems.

Excellent teachers use varying lecture styles that actively engage students in the learning process. Information technology also allows a pure lecturing format to be supplemented or in some cases replaced by an integrated lecture/laboratory situation. In this mode the instructional material is presented on the computer with the conceptual elements explained and supplemented by the instructor's lecture. At the end of the presentation, a laboratory exercise is executed on the computer under the supervision of the instructor to give experience in application of the concepts or processes (see www.center.rpi.edu/PewGrant.html for examples). The interactive mode of intermingled lecture and laboratory has a very high reinforcement value. The computer system is used to mediate the rate at which information is presented to each individual student.

In the so-called "studio" approach, the lecturer can move among the students, looking over their shoulders and serving as an advisor and facilitator. Teaching and learning becomes more a one-on-one or small group exercise and less a remote lecture exercise. The instructor thus is transformed from being a "sage on a stage" to a "guide on the side". This integrated lecture/laboratory mode of instruction is now being used in industrial training, particularly in the software industry. Learning and cognitive studies have shown definitively that personalized learning via immediate feedback has a significant impact on retention.

An extension to the use of technology in the discussion is distance education, which is the combination of technology-based education with technology-based delivery of a complete course. Distance education has been defined as any formal approach to learning in which a majority of the instruction occurs while educator and learner are at a distance from one another. Anyone who has listened to a Pavarotti CD but never heard the great tenor in person has certainly received a certain level of enjoyment (and perhaps inspiration) from this great singer, even though the interaction is not face-to-face.

Distance education appears to be a good fit for continuing education, where highly motivated, mature students make sure they learn what is needed. Having such classes offered at a convenient time and place (asynchronous mode) is critical for professionals with full-time jobs, who need to update their skills and knowledge base in response to changes in the economy. The availability of streaming media technology (audio and video) over the Internet eventually will make delivery of courses to personal desktop computers an economic reality. The faculty member's office then becomes the studio, which will make educational delivery at lower cost than with the interactive television mode currently employed at many universities. This may suggest the merging of this approach with the traditional classroom, leading to hybrid lecture/distance education courses.

The Interactive Authorship

By James B. Riggs
Department of Chemical Engineering
Texas Tech University
Lubbock, Texas 79409-3121

The established paradigm for authoring university textbooks is to develop a manuscript, obtain a contract with a publishing company, edit the proofs of the text, wait for the yearly royalty check, and complain that one receives less than minimum wage for the time that was spent writing a textbook. Large publishing companies generally receive over 80% of the gross profits from a textbook while contributing only 10% to 20% of the overall effort and providing about one-third of the initial overall investment (considering the value of the author's time for developing the manuscript). In addition, publishing companies sell textbooks generally with little interaction with the professors that use them. With the advent of powerful and easy-to-use publishing software and the relatively low cost associate with printing a book, self-publishing textbooks have become a viable option that eliminates the middleman -- namely, the publishing company -- between the author and the college bookstore. Self-publishing a textbook allows authors to realize all the profit from their books, control the quality of the production of the textbook, and determine and implement the marketing strategy for the text. In addition, a real opportunity for self-publishing authors is to provide personal interaction, supplementary materials and services to the professors who have adopted their textbook that can improve the performance of the textbook in the classroom.

Software companies have done an excellent job of providing service to their customers by being sensitive to their needs. They recognize that their business is largely dependent on meeting the needs of their customers and that their customers are the best source of ideas for developing new software products. They actively solicit input form their customers on the effectiveness of their products based on the customers experience with the software. The good software companies get in the "trenches" with the customers to more fully understand the needs of the customers and use this experience to develop improved products. They understand that they are in a service business, i.e., serving the needs of their customers.

I believe that the university textbook business should be a service industry as well even though the publishing companies have not treated it that way. The approaches presented here are means of providing service to the professors that use the textbook, are a means of develop material for future editions of your text, and are effective ways to retain your customers. This approach is referred to here as an interactive authorship since it is based on different ways of interacting with the customers, the professors that are using the textbooks in their classes.

The interactive authorship can include, but is not limited to (a) sharing course materials; (b) sending out questionnaires to professors and students that are using the textbook; (c) using follow-up calls or email exchanges to the professor; (d) acting as a clearinghouse for sharing exams and projects among the adopting professors; and (e) disseminating new material as soon as it is ready for distribution.

Sharing Course Materials

Supplementary material, such as simulation software, the solution manual, electronic lecture slides, and lecture notes, is material that you might develop for your course to facilitate the class. As a self-publishing author, you can share this material with the professors that have adopted your textbook and professors that are considering adopting it with very little additional effort. Sharing this material will make it easier for professors to switch to your textbook and make it easier to keep the adoptions that you have. In each case, the supplemental material is most efficiently distributed by email since you should develop the necessary distribution lists from your marketing effort.

Simulation software. For textbooks in science and engineering, simulation software can provide an effective compliment to a textbook. Simulations can provide a "hands-on" experience for students that can greatly increase the student's understanding and working knowledge of the subject.

There are a variety of formats that simulation software can be provided for. For example, computer programs can be developed in standard programming languages, such as Basic, FORTRAN, C, C++, Pascal, etc. The standard versions of these programming languages do not have convenient graphical interfaces for them; therefore, students would have to develop their numerical results and transfer them to a graphical program to view the results. This is a less than satisfactory offering in the era of point-and-click.

Visual versions of most programming languages, such as Visual Basic and Visual FORTRAN, are available and allow the student to more conveniently display the results as they are calculated by the program. Using these programs, you can generate very attractive color displays with a menu driven format requiring no programming skills from the student.

There are also software packages, such as MatLab, that offer numerical solution functions and graphical display capability. These packages are really high level programming languages, but they are usually much more user-friendly than standard programming languages, such as FORTRAN.

Chemical engineering faculty have also created a variety of application-specific software; examples include Control Station by Doug Cooper and Polymath by Mordechai Schacem and Mike Cutlip, the latter being marketed by the CACHE Corporation.

You may also want to develop a windows version of your simulator in which the user clicks the appropriate boxes on a file page and based on their requests new choices and input data requests show up on the screen. After the simulator has been provided all the necessary input data by the student, the graphical result are displayed. You can develop some attractive and functional software that provides new experiences and insights for the students using the aforementioned software, but it will take a significant amount of time to learn how to use this developmental software to produce the kind of simulation software that you want. Disciplines other than engineering and science can develop software programs that assist the student to learn the material. These learning modules are, in effect, the same as simulators.

Solution manuals. If you have homework problems, questions, discussion questions, or projects in your textbook, you should develop a solution manual. If a textbook does not come with a solution manual, the adopting professor will have to put a lot of extra work either into grading his homework or into developing a solution manual for the teaching assistants to grade the homework. As a result, some professors insist on having a solution manual for a textbook before they will adopt it for their class.

The solution manual can either be a paperback book or it can be in an electronic form. The solution manual can be developed using your publication software and printed to paper to develop the master copy for the paperback version or it can be converted to an Adobe Acrobat PDF file for the electronic version. The paperback version can be produced using your local copy shop since you will not need a large number of copies. You should only need 20 to 30 hardcopies of the solution manual to start with. Most professors will be happy with an electronic version. The electronic version can be conveniently sent out by email, thus avoiding the copying and the mailing costs, so that it arrives faster.

The electronic version of the solution manual can be used to provide the solutions to the homework and unassigned problems to the students after their homework has been submitted. This can be done by posting a read-only PDF file on the web page for the course on a chapter-by-chapter basis. Adobe Acrobat 4.0 provides security protocols for generating PDF's that will prevent all but the most creative and industrious students from copying them.

Electronic lecture slides. Electronic lecture slides have become a popular method for classroom presentations. They can be shown to a class by using a laptop computer, which has files containing the electronic slides stored on them, that is connected to a special projector. Attractive lecture slides with a wide variety of artwork can be easily developed using user-friendly software. Moreover, since you will have access to the original artwork for your textbook, you can use this resource to develop quality slides that have the same graphics that are used in the textbook. For example, I developed a set of 400 lecture slides in about 80 hours of effort that covered a semester's worth of material for my undergraduate control class.

I like to use slides for my lectures because it provides a convenient framework to lecture from. That is, it provides an outline to follow and I do not have to spend a large portion of the class time drawing schematics and plots. In addition, the slides can be provided to the students. For example, the slides can be copied 6 to a page on the front and back of the page and supplied to the student, or the students can be given access to the electronic version of the slides and they can make their own copies. In either case, if they come to the lectures with the slides, they do not have to try to reproduce all the presentation material, including the artwork, and they can concentrate on developing an overview understanding of the material. That said, it should be pointed out that some studies have shown that hand written board presentations are more effective than slide presentations. This is probably true for presentations involving derivations since for board presentations the student would have to copy the derivation by hand. If you subscribe to the argument that students learn more by writing the lecture material, then do not make the slides available to them.

Electronic slides can be developed using several commercial presentation packages including Microsoft Power Point and Corel Presentation. Each of these comes with a number of slide formats, patterns, and colors. In addition, they are available with several options, including slides that are built piece-by-piece as you go through the slides and interesting transitions between slides. When you need to make additions or corrections, it is an easy matter to do so; therefore, electronic lecture slides are a work-in-progress and tend to evolve as you use them.

Lecture notes. Lecture notes contain the material for classroom board presentations that include organized text materials and graphical material. Providing professors with this material would greatly reduce the amount of work that they would have to do in order to develop their lecture notes. Even though most professors would not use the unaltered version of these lecture notes for their lectures, they could use them as a starting point for developing their own set of notes. In this manner, they can be sure that they have considered all the relevant topics and they can still insert additional material as they see fit and reorganize where necessary.

The lecture notes can be developed using publication software using the artwork from the book as needed. Therefore, the lecture notes can be converted to PDF files and distributed by email to the adopting professors and the professors that are considering the textbook for possible adoption.

Questionnaires

Questionnaires are a convenient means of obtaining feedback from professors and students as to their experiences with using your textbook in their class. Designing a questionnaire is not as simple as it might seem. One must be careful to phrase the questions so that the most useful information is obtained. In general, it is probably best if you ask both specific and general questions so that you get feedback to specific issues and you allow the responders to say what is on their mind. For example, a general question might be to ask what the reader likes or dislikes about the textbook.

Email is an efficient means of distributing the questionnaires. Once you learn that a department has adopted your book for their class, you should add the email address of the professors that teach the class in the adopting department to a distribution list. A separate distribution list should be developed for each semester/quarter so that the questionnaire is only sent to professors that are currently using your textbook for their class. A questionnaire for the professors and a separate questionnaire for the students can be developed using a standard word processor, such as Microsoft Word. Then send an email message to the proper distribution list with separate questionnaires for the professor and the students attached. The message in the email to the professor should request that they complete the professor's questionnaire and have their students complete the student's questionnaire and that they please return the questionnaires to you. In addition, you should also mention in the message how the results of the questionnaire will be used and why it is important to you to have that information. In this manner, you can send out one email and generate a survey from all the professors and students that are currently using your textbook. The professors that receive your questionnaire can forward the responses to you by email or they can make hardcopies of the questionnaires and return the questionnaires by “snail-mail”. Do not expect 100% participation, professors are very busy professionals. In fact, my limited experience with email distribution of questionnaires is that I received only a 15-20% response rate, i.e., only one out of five or six professors contacted will actually respond. Nevertheless, this sample can usually give you a clear idea of the strengths and weaknesses of your textbook and identify areas where you text can be improved. Clearly, when you receive the same criticisms from independent sources, it must be taken seriously. In addition, some professors may provide explicit feedback including the types of material that should be included and even specific descriptions of examples or problems.

Follow-up Calls to Professors

Many of the professors will not find the time to complete their questionnaire, distribute the questionnaires to the students, and return the results to you; therefore, it is advisable to contact the professors who do not respond by phone to solicit their feedback. The best time to contact them is after their semester/quarter is complete. Some of the professors that you contact may be reluctant to criticize a textbook to the author so you may have to probe them a bit to get an honest opinion. It is probably helpful to mention that it is important for you to learn what the professors using your text disliked about it if you are going to be able to improve it in the future. These discussions can be built on a sense of cooperation between the professor and the author if the communications are open and honest. Clearly, an author should guard against being defensive about criticism of his book if he expects to receive useful information. Remember that what you are hearing is just one person’s opinion and do not try to change it. Instead make sure that you understand clearly what faculty adopters are saying. This can be difficult since most authors are emotionally attached to their books, but you must remain detached from the criticism if you are going to be able to factor out the important information in a critical or even heavy-handed assessment of your book. All feedback should be considered, but remember that when you start hearing the same feedback from independent sources, it is time to take it more seriously.

Clearinghouse for Shared Exams, etc.

Most professors put a lot of thought and effort into developing their exams. They have to decide what is important enough to test and how to test it. As a result, it can be difficult to create new exams each year that are stimulating and test the knowledge and creativity of the students. Since self-publishers following the approach presented here maintain email contact with the professors using their textbook, the self-publishers can serve as a clearinghouse for an exchange of exams between the adopting professors. In this manner, each participating professor can **anonymously** share an exam with the group and in turn receive copies of all the exams collected, which can be quite a resource of questions, problems, and ideas. While this resource should benefit the professors who participate, the collection of shared-exams is a great resource for problem types and approaches for the authors for future editions of their textbook.

The approach that I used was to send an email to all the professors using our textbook explaining the request and the value of such a resource and indicating that only those professors that send at least one exam would receive the collection of exams.

Therefore, all the professors had to do was reply to my email and attach one or more exams to the reply which should only take a couple of minutes if they have an electronic version of one of their exams. I had over half of the professors that use our control textbook respond affirmatively to this request and I received over thirty exams. Some of them were hard copies so I had them scanned into separate PDF files so that the whole collection was available electronically. At the same time I built a distribution list for those who chose to participate in the exam clearinghouse. In a couple of weeks after I had received all the exams, I sent an email using the exam clearinghouse distribution list to all the participants with the copies of the exams attached. During the follow-up calls, I reiterated the offer to participate in sharing exams and since it was after the semester was over, a number of them decided to participate thereby further increasing the size of the exam collection.

This approach is not limited to the exchange of exams. The self-publisher can promote the exchange of all types of materials and approaches used in conjunction with teaching the class. For example, the self-publisher using the same clearinghouse approach can promote an exchange of course syllabi, laboratory approaches and experiments, class projects, and homework problems. In addition, the self-publisher can establish and administer a forum on the internet for students to exchange their studying approaches, experiences, and anything associated with the course with students from other universities using the same textbook. The forum could be an opportunity for the authors to develop new insights into the attitudes and approaches of the students to their textbook and university study in general.

Dissemination of New Material

Since self-publishers are exposed to a wide range of ideas from the feedback on their textbooks from questionnaires and follow-up calls as well as from the collection of shared-exams, it is likely that they will develop new materials based on these ideas for their own classes. These materials should compliment the textbook while expanding and improving the materials used by the class. These materials may also be the basis for modifying the textbook for a new edition. As these materials are developed, it is convenient to distribute them by email to the professors using the textbook. This will serve to improve the materials of the professors using the textbook and may solicit feedback on the materials by those who use them.

Clearly, since the interactive authorship generates new ideas from an exchange of materials and from quality assessments of your textbook from your customers both of which can be used to develop new materials that can be quickly distributed, it is an effective means of improving the quality of your textbook while enhancing your ability of retaining adoptions.

Self-Publishing Economics and Logistics

The table below lists the net income for self-publishing and for using a large publishing company to publish a 500-page black and white engineering. In addition, all the factors necessary for calculating the net profit are listed: retail price, wholesale price, initial printing costs, initial marketing costs, net profit, and assumed market sizes. This table is based on printing 1000 copies of the text in the first printing of the book. The larger the print run, the lower the printing cost per book, but the larger the initial capital investment, e.g., 2000 copies would cost about $5 per copy. An initial print run of 1000 copies is a reasonable initial print run based on compromise between these factors.

This table is also based on using a 20% discount rate for calculating the wholesale price. The materials of construction and the construction procedures were appropriate for the different textbook markets. You can easily see that increasing the cost of the printing of a textbook by 10% to 20% has a relatively small impact on the net profit of a self-publisher. Certain students sell their textbooks back to the bookstore at the end of the semester. The percentage of the books that are sold back to the books store has a significant effect on the profitability of a textbook and it will depend on the how the student perceives the utility of the textbooks for future use.

While there are number of assumptions in this table, with the market size and percentage of the market captured being the most important and the most uncertain, these results should be representative of a large number of textbook markets. In any event, note that the ratio of self-publisher income to royalty income ranges from about 5 to almost 7. In other words, if you choose to self-publish and you only do as good as a publishing company in terms of sales, you can expect to make 5 to 7 times as much as you would have if you had used a publishing company. The incremental effort required to perform the publishing activities is usually only 10% to 20% of the effort required to write the textbook. Market size, sale price, the percentage of returns, and production costs can vary widely depending on the particular textbook market, but you can easily used this table as a template to estimate the potential profitability of your own textbook project.

Based on these examples, consider how many books would have to be sold to recover the initial capital investment, i.e., the cost of printing 1000 copies and the initial marketing cost. For the engineering text, the number of sales required to recover the initial investment is 111. Therefore, it should not very difficult to at least recoup the initial capital investment.

	EngineeringTextbook
Type of Binding	Hardbound
Number of Pages	500
Retail Sales Price	$90
Wholesale Price	$72
Printing Costs per Book	$7
Marketing costs per Book	$1
Profit per book	$66
Percent Returns	20%
Total Market Size (Books per year)	4000
Annual Profit for Self-Publishing	
10% of the market	$23,000
20% of the market	$46,000
30% of the Market	$69,000
Annual Profit for 12% Royalty	

10% of the market	$3500
20% of the market	$7,000
30% of the Market	$10,000

Conclusions

Self-publishing textbooks facilitates a service orientation for textbook publishing that should provide materials that assist students in learning and professors in teaching while providing the authors with new and diversified ideas for improving their textbooks. Due the efficiency associated with e-mail, Internet access, and powerful new software, the interactive professorship approach is a highly effective activity when you consider the results obtained for the time invested.

A more complete description and analysis of self-publishing university textbooks can be found in the following book:

A Guide to Self-Publishing University Textbooks
(www.ferretpublishing.com)
By
James B. Riggs

Abstract

The established approach to authoring a textbook today is based on contracting with a large textbook publishing company. That is the author develops the manuscript and sometimes the artwork and relies on the publishing company to produce, market, and deliver the books to customers. Publishing companies receive over 80% of the gross profits from these arrangements leaving the rest for the author. On the other hand, the author tend to provide 80% to 90% of the overall effort and easily exceed the investment by the publisher if you count the value of the author's time spent developing the manuscript.

With the advent of desktop publishing, another alternative exists for the author of university textbooks, i.e., self-publishing. That is, due to the availability of personal computers and the development of powerful publication software, university professors can effectively and efficiently eliminate the use of a publisher by becoming their own publisher. Self-publishing a successful textbook can increase the income from the book for the author by a factor of 5 to 7 compared with the traditional royalty from a publisher. The additional effort required for self-publishing amounts to 10% to 25% of the effort required to write the textbook depending on how involved in the publishing business portion that the author decides to be.

Self-publishing a textbook involves developing the manuscript and artwork, typesetting the book, working with a printer to manufacture the books, and marketing and fulfillment to the customers. A clearly written and well-organized manuscript that is relatively error-free, is easy to use, and provides the proper coverage of the material is a prerequisite for a successful textbook. It is probably more efficient to develop your

manuscript directly on the publication software that you have chosen for typesetting. In addition, the artwork for the textbook can be developed using software designed to develop schematics, line drawings, and digital versions of photographs and the artwork can be imported into the typeset pages of the textbook. While finishing the manuscript, you should choose the materials of construction and select the printer who will manufacture your inventory of books. When the manuscript is complete and typeset, an electronic version of the book should be sent to the printer.

Aside from the quality of the manuscript, marketing is the most important factor affecting the success of a self-published textbook. At about the same time as your manuscript is sent to the printer, you should begin your marketing effort by designing a brochure and having it printed so that you can begin sending the brochure to the proper university departments a few weeks before you expect your books to return from the printer. Marketing can be viewed as two primary activities: (1) getting exam copies into the hands of the professors that make adoption decisions and (2) making sure that these professors understand the key attributes of your textbook. The primary methods for accomplishing these tasks are mailing promotional brochures and telemarketing to the target professors. Other techniques compliment the primary marketing approaches and include e-mail marketing, Internet advertising, journal book reviews, displaying the text at conferences, and direct visits.

The self-publisher can also conveniently interact with the professors and student using his book due to the capabilities of the Internet and e-mail. The interactive authorship involves (a) sharing course materials; (b) sending out questionnaires to professors and students who are using the textbook; (c) using follow-up calls and email correspondence to the professor; (d) acting as a clearinghouse for sharing exams and projects among the adopting professors; and (e) disseminating new material as soon as it is ready for distribution. It is an effective means of providing services to your customers (i.e., the professor and students that use your book) and thereby improve your retention rate while developing quality new materials for future editions of your book.

Similar to other businesses, establishing a self-publishing business involves a number of financial, legal, and day-to-day business activities. One of the most important financial activities is raising the capital required for the initial printing and marketing effort. There are a number of issues associated with operating a self-publishing business including setting the retail price of your textbook, determining the discount rates, setting the terms of sale, choosing a return policy, managing your inventory, recording your expenses for documentation of your tax deductions, planning for your business taxes, and fulfilling book orders and orders for exam copies. Electronic versions of textbooks (e-textbooks) may become popular in the future due to several attractive features, but they must overcome security issues and a general lack of experience with this form of textbooks.

Table of Contents

Chemical Microengineering. I. Introduction

By Peter R. Rony
Department of Chemical Engineering
Virginia Tech
Blacksburg, VA 24061-0211

What is Chemical Microengineering?

Chemical microengineering is defined as the study of the engineering of small chemical systems. A chemical system is defined as being "small" if at least one coordinate direction, and usually two, has/have a size smaller than one millimeter. Such systems are much easier to mathematically model than the 3-D equipment in typical large-scale chemical systems.

As taught at Virginia Tech starting in 1974, ChE 4114 is a senior elective course in chemical microengineering that includes the study of (a) the continuity-of-species equation for "small chemical systems"; (b) clever ideas and interesting gimmicks that are used in small chemical systems; and (c) interesting molecules.

Examples of Small Chemical Systems

Some examples of "small" chemical systems include:

- A biological cell in any living organism
- A leaf of a plant
- A root hair on a plant
- A sac in a human lung
- A glomerule in a human kidney
- An ion-exchange pellet
- A pellicular absorbent inside a packed, gas-liquid chromatographic column
- The thin liquid film inside a capillary chromatographic column
- An enzyme immobilized on a porous support
- A supported liquid-phase catalyst pellet
- A hollow fiber enzyme reactor
- An ion-specific electrode
- A hollow fiber
- A microcapsule
- A microdroplet within a microemulsion
- An aphron

Though a plant leaf can have a large surface area, the small leaf thickness places such a system into the chemical microengineering category. Though a capillary chromatographic column can easily exceed 10 meters in length, the small thickness of the adsorbed liquid film inside the capillary also places such a system into the chemical microengineering category. A biological cell is the finest example of a small chemical system.

To repeat: the rule of the game in chemical microengineering is that one or two coordinate dimensions of a specified chemical system is/are smaller than one millimeter in length. The list of small chemical systems is almost endless.

Quote No. 1: Basic Phenomena of General Applicability

In the context of chemical microengineering, a favorite quote is from Paul B. Weisz [2]:

> ***"We have traced the significance of the competition between molecular reaction and molecular diffusion, as expressed by the Phi criterion, across many disciplines. It is interesting to note how researchers in many branches of the sciences have struggled with problems that arise from a basically common phenomenon, one that does not "belong" to any special discipline. We need to consider how we might best prepare ourselves and our students to understand and deal with basic phenomena of general applicability. While we continue a healthy trend to erase interdisciplinary boundaries, we must remember that any collection of items as complex as those that constitute human knowledge can only be sensibly stored, managed, or propagated with some unifying structure. Can we find structures that are orderly, basic and interdisciplinary? Can the teaching of human experience and knowledge be organized around phenomena? The diffusion-transformation interaction is but one example of a general phenomenon: there are many others. . . . each represents a general concept or phenomenon that has meaning, implications, and applicability across an enormous sector of experiences and disciplines: physical, biological, social, physiological, medical, psychological, and others. Furthermore, each can be experienced, enjoyed, and understood in some form at nearly every stage of educational development."***

"Chemical Microengineering" is a course that responds to Dr. Weisz's challenge. But what phenomena would be appropriate for such a course?

Quote No. 2: Processes are Not More Complicated Than Things

Edward De Bono [2] suggests an answer:

> ***"Up til quite recently, the world was full of things. That is to say, the most useful and respected way to look at the world was in terms of static things. These things were given very definite names and fitted into great schemes of categories and classifications and sub-classifications. Every thing had its proper place and, being a static thing, it stayed there."***

> ***"It is often felt that processes are much more complicated than things. I do not believe this is so at all. It is true that you can see cars and bicycles and boiled eggs every day, but rarely see polarization or feedback or pattern. But this may only be because one has never learned to look for them. It can be just as much fun to look for feedback in daily life as it is to look for snails in the garden or buttercups on a country wall. And one can become just as quick at recognition."***

De Bono's first list of process concepts includes the following items:

> ***"to feedback***
> ***to manage***
> ***to forecast***
> ***to optimize***
> ***to control***
> ***to permit***
> ***to catalyze***
> ***to transfer***
> ***to convert***
> ***to sample***
> ***to oscillate***
> ***to filter***
> ***to polarize***
> ***to trigger off***

to extrapolate
to amplify
to regenerate
to communicate"

Quote No. 3: Some Phenomena and Processes in Chemical Microengineering

In chapter 4 of a supplementary ACS "sourcebook for physical chemistry teachers", Rony suggests the following lists of phenomena and processes [3] for a chemical microengineering course:

> ***"In the spirit of the comments of Weisz and de Bono, what are the phenomena and processes associated with applications of the continuity-of-species equation? First are the processes, which can be expressed as verbs:***
>
> ***to diffuse***
> ***to distribute***
> ***to convect (to undergo convection)***
> ***to partition***
> ***to separate***
> ***to react***
> ***to catalyze***
> ***to accumulate***
> ***to undergo a diffusion-controlled reaction***
> ***to equilibrate***
> ***to undergo a convection-controlled reaction***
>
> ***"Second are the phenomena, which can be expressed as nouns:***
>
> ***diffusion***
> ***partitioning***
> ***convection***
> ***separation (diffusion-controlled convection)***
> ***reaction (chemical kinetics)***
> ***accumulation***
> ***catalysis***
> ***equilibration***
> ***diffusion-controlled reaction***
> ***distribution***
> ***convection-controlled reaction"***

In chemical microengineering we demonstrate an intellectual framework in which a discussion of such phenomena and processes can occur naturally. Such topics are also appropriate in a physical chemistry course, which is why chapter 4 was written for the 1988 American Chemical Society sourcebook for physical chemistry teachers.

Example Categories of Clever Ideas and Gimmicks

In addition to identifying appropriate chemical microengineering processes and phenomena, we have also identified an eclectic group of principles that we call "chemical microengineering gimmicks":

- 2-dimensional equilibria
- Linear multistate chemical systems

- Pulse chromatography
- Affinity chromatography
- Gel permeation chromatography
- Porous solids/high interfacial areas
- Molecular anchoring
- Molecular barriers
- Molecular arrays
- Molecular recognition
- Extent of separation index
- Diffusion-controlled reaction
- Convection-controlled reaction (reactor)
- Dimensionless groups
- Catalysis
- Molecular carriers and facilitated diffusion
- Molecular isolation
- Molecular confinement
- Molecular protection
- Molecular inhibition
- Molecular bookkeeping
- Timed-release
- Countercurrent flow
- Combinatorial chemistry
- Short diffusion path lengths
- Use convection rather than diffusion to move molecules
- Microcapsules
- Microemulsions
- Aphrons
- Hollow fibers
- Liquid membranes
- Molecular tags
- Molecular amplification
- Molecular oscillators
- Molecular self assembly
- Molecular layers
- Molecular feedback
- Nanotubules
- Molecular sieves
- Molecular sensors
- Oscillogenic instruments

Example Categories of Interesting Molecules

The skills of chemists in creating interesting molecules is accelerating. Such molecules can be organized according to the categories of molecular topology, molecular machines, and molecular electronics. Molecular topology provides the greatest selection of interesting molecules, which include:

- Molecular cages (clathrates)
- Molecular claws (chelates)
- Molecular tubes

- Molecular geodesic domes
- Molecular channels
- Molecular separators
- Molecular spirals

Possible examples of molecular machines include:

- Molecular brushes
- Molecular zippers
- Molecular bearings
- Molecular drills
- Molecular handles
- Molecular chains

The synopsis to the article, "Computing with Molecules", by Reed and Tour [7], reads as follows: ***"Researchers have produced molecules that act like switches, wires and even memory elements. But connecting many of the devices together presents enormous challenges"***. A remarkable figure from this article is the plot of Conductance (0.00 to 0.10 microSiemens) versus Voltage (-5 to +5 Volts) for a single benzene para-dithiol molecule bonded between two gold tips. The molecule could sustain a current of approximately 0.2 microAmpere at five Volts, or Teraelectrons per second in single file through the benzene dithiol. Although more complex logic circuits may be difficult to create, single molecules that exhibit the following examples of molecular electronics may be possible, even likely, to synthesize"

- Molecular switch
- Molecular diode
- Molecular conductor
- Molecular superconductor
- Molecular memory
- Molecular transistor
- Molecular wire
- Molecular amplifier
- Molecular address
- Molecular AND gate
- Molecular OR gate
- Molecular RAM
- Molecular ROM
- Molecular communications

Why Now?

The author has observed a significant evolution of research interests in the Virginia Tech ChE department, between 1970 to 2000, probably typical of research trends in ChE departments nationwide. In 1970, the focus of research was on traditional, chemical engineering topics, most of which had a negligible chemistry or biochemistry component. By 2000, at least two-thirds of the Virginia Tech faculty are engaged in research projects that have a chemical-microengineering flavor. It is likely that this trend in research interest will filter down to the undergraduate curriculum.

Quote No. 4: Microengineering Beyond the Electronics Domain

Another favorite quote is from Thomas Hirschfeld [5]**:**

"Mainly, however, microengineering beyond the electronics domain gives us the possibility of designing objects in an entirely new fashion since the significance of the physical and chemical principles involved changes as the scale of the system decreases. In an attempt to learn from experience, we have kept in mind that the biological world has been designing on the micrometer scale for eons and, thus, furnishes us with some impressive examples of microengineering. . . .

"We have undertaken a systematic study of the physics, chemistry, and engineering of the microscopic domain. To do this, we have had to bring together a number of fields that initially do not appear to have much in common. The obvious starting point was microelectronics and its fabrication technology. However, unless we were to build everything out of silicon and only in two dimensions, we could not stop there. We soon realized that microscopic sizes are the normal design range of the biological world, and, after a billion years or so, nature has accumulated considerable expertise in this area. Through a careful search of the molecular biology and entomology literature, we identified a number of useful biological devices and design principles that can be incorporated in our microengineered devices.

"This leads directly to the first major technical task in microengineering-identifying the scaling laws. The scaling laws describe the variation in the relative importance of different phenomena as things change in size. For example, weight increases with the cube of a linear dimension but strength increases only with the square. . . ."

Quote No. 5: The Century of Biology

Equally appropriate here is a quote by John Carey [6]**:**

"New research technologies are vastly accelerating the pace of discovery in biology, driving forward not only medicine but also industry, environmental cleanup, and agriculture. Scientists are unlocking biochemical pathways in cancer, clogged arteries, and Alzheimer's disease. Not only are they understanding life, they're manipulating it. They are slipping new genes into people to treat disease and genetically engineering plants and animals to boost yields or transform them into bio-factories of plastics and drugs.

"Add it all up, and just as information technology undergirds today's booming economy, biology may drive tomorrow's. In fact, biology could transform information technology through such developments as DNA-based computers and software that repairs flaws as nature does. ''We are now starting the century of biology,'' says J. Craig Venter, president of the Institute for Genomic Research and pioneering gene finder."

Clearly, the biological-system-based component of the 21st-century chemical engineering curriculum, will need to significantly expand from its current base of almost zero. One example of such expansion is the inclusion of a semester or two of biochemistry, perhaps supplemented by a biochemistry lab course.

A course in chemical microengineering provides an additional opportunity to discuss important principles of biological systems in the context of chemical engineering.

Cross - Fertilization Between Chemistry and Chemical Engineering

The author participated in a 1980 workshop on "Cross - Fertilization between Chemistry and Chemical Engineering", sponsored by the ACS Education Commission, ***"which expressed concern about introductory physical chemistry courses and recommended that a study of the situation be made."*** The author contributed the 36-page Chapter 4 to the resulting product of this workshop, namely, a paperback ACS publication entitled "Essays in Physical Chemistry:

A Sourcebook for Physical Chemistry Teachers" [3]. One day, the typical physical chemistry course may incorporate topics related to the continuity-of-species equation. The topic is as relevant to chemists as are other physical-chemistry theoretical topics, including quantum mechanics, statistical mechanics, chemical kinetics, and thermodynamics.

What Next?

This article is the first of a series of planned articles in CACHE News Online that explore various aspects of a Chemical Microengineering senior elective course for undergraduates. The author has taught such an elective course, off and on, since 1974 with the hope that it would attract a multidisciplinary undergraduate audience. In 26 years, the course's single interdisciplinary student was Dr. Yoel Sasson, a post-doctoral researcher from the Hebrew University of Jerusalem. Dr. Sasson learned the principle of phase-transfer catalysis during the 1970's version of the chemical microengineering course, and has become since that time an international expert on the subject [8].

Subsequent CACHE News Online articles will explore items from the listings contained in this paper.

References

1. Paul B. Weisz [Science magazine 179 (4072), 433-450 (1973).
2. Edward De Bono, Chemtech 2, 456 (1972).
3. Peter R. Rony, "Continuity of Species in Physical and Chemical Processes", "Essays in Physical Chemistry", W. T. Lippincott, Editor, American Chemical Society, 1988, pp. 29-64.
4. Computers in Chemical Engineering Education, Brice Carnahan, Editor, CACHE, 1996.
5. Thomas Hirschfeld, “Providing Innovative System Monitoring and Reliability Assessment Through Microengineering”, Energy and Technology Review, Lawrence Radiation Laboratory, Livermore, CA, (internal publication), (February 1984) p 16.
6. John Carey, "We are now starting the century of biology", Business Week (August 21, 1998).
7. Mark A. Reed and James M. Tour, "Computing with Molecules", Scientific American **282**, 86-93 (June 2000).
8. Yoel Sasson aand R. Neumann, Editors, "Handbook of Phase Transfer Catalysis", Blackie Academic & Professional, London, 1997.

ENGINEERING AND COMPUTATIONAL ISSUES IN INDUSTRIAL BIOLOGY

Implications for Commercializing Biology in the 21st Century

Babatunde Ogunnaike
DuPont CS&E

1. INTRODUCTION

- AN ENDURING PARADIGM
  - ➢First, Science, *then* its commercialization;
  - ➢Technology–the enabling “middleman”;
  - ➢Inexorable driving force: meeting societal needs

Evolutionary Trends?

- 19th Century
  - ➢Science: PHYSICS
    - ◆ Origin in Newton's 18th Century;
    - ◆ Spilling over into 20th Century;
  - ➢Commercialization
    - ◆ from Edisonian light bulb to locomotive engine, to refrigeration, to skyscrapers …
  - ➢Enabling Technology: (Mech.) Engineering

Evolutionary Trends?

- 20th Century
  - ➢Science: CHEMISTRY
    - ◆ with significant influence from Physics;
  - ➢Commercialization
    - ◆ modern chemical industry, still viable, but in need of re-energization…
    - ◆(Late dominance of “Parallel Universe” of “Electronics” arising from *integrating Physics*)
  - ➢Enabling Technology: (Chem.) Engineering

Evolutionary Trends?

- 21st Century
  - ➢Science: BIOLOGY
    - ◆ with significant influence from Physics *and* Chemistry;
  - ➢Commercialization
    - ◆Ongoing “gold rush”…
  - ➢Enabling Technologies: Still evolving
    - ◆Tantalizing observation: *any fundamental connection between “Information” and “Cells”?*
- Any clues from the past?

Issues to Consider

- “Proximity” of the Science to the relevant Engineering.
  - ➢How far does the “enabler” have to travel?
- Tools of the Engineering trade
  - ➢What is needed? Is it available?

2. COMMERCIALIZATION

- What is going on?
  - ➢Biology Research Drivers
  - ➢Biology R & D Activities
- Engineering Involvement

Biology Research Drivers

NIH funding ($15.6 billion in 1999, 82% extramural)

Pharmaceutical Industry(est. $26 billion U.S. R&D 2000)
-part of healthcare - largest market segment
-huge unmet needs - cancer, aging, heart disease
-most profitable industry
-highest investors in R&D as percent of sales
-baby boomers will pay anything to stay young forever

Agriculture ($X billion R&D)
-world population now 5E9 will be even higher in 2030

Materials ($Y billion R&D)
-sustainable alternatives to oil
-higher value products

Activities of Biology R&D

Laboratory work

hypothesis testing (drug target validation)

data generation (to discover new genes)

Hypothesis generation *(deep thinking by scientists/domain experts)*

"..we propose that stabilizing selection has maintained phenotypic constancy for *eve* expression but has allowed mutational turnover…"

Data organization

assembling genomes (human has 3E9 bases, ~140,000 genes)

Data analysis

developing and testing algorithms for recognizing genes and their control elements in DNA sequence

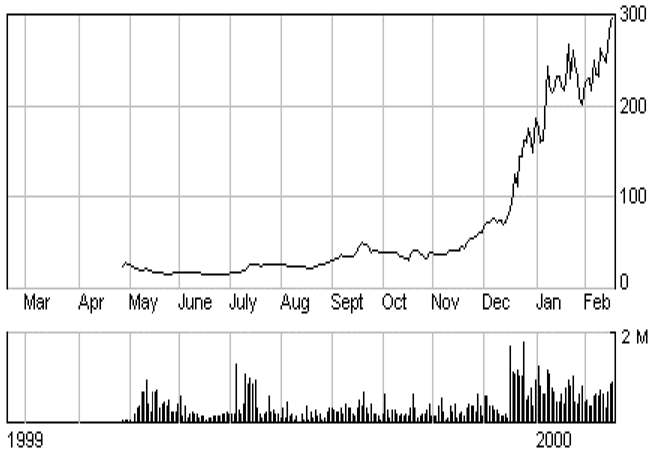
Technique development

new ways to turn genes off and on experimentally

Highest Value Activities Currently

High throughput data gathering, organization, analysis
For example 2 companies with IPO's last year:

Celera Genomics ($8.2E9 mkt. cap)
faster sequencing,
first to finish human genome



Curagen Corporation ($3.6E9 mkt. cap)
first to map protein-protein interactions
for an organism (yeast)

Engineering-like activities

Industrialization of Biology:

Celera -- old sequencing machines, new machines
Curagen -- industrialized gene expression measurement with gels, now industrializing 2-hybrid assay.

Both cases:

Machines/robotics to aid data generation
Computer software to organize, search, analyze, present data

Involvement of Engineers

Not intense domain knowledge of expert;
Understand generic molecular biology;
Know promising new techniques;
Be first to scale-up techniques;
Have expertise in computer technology --

web tools, databases, interfaces, algorithm design
(industry average for bioinformatician is $94K/yr)

Future Targets for Engineers in Biology

- Invent important techniques and methods
- Models of biological systems -- make biology predictive
  - ➢Entire cells, Diseases (cf. Entelos, Inc)
- Invent in “Molecular Biology” too?
  - ➢ See Yeast 2-hybrid (*Nature*:**340**,1989)!

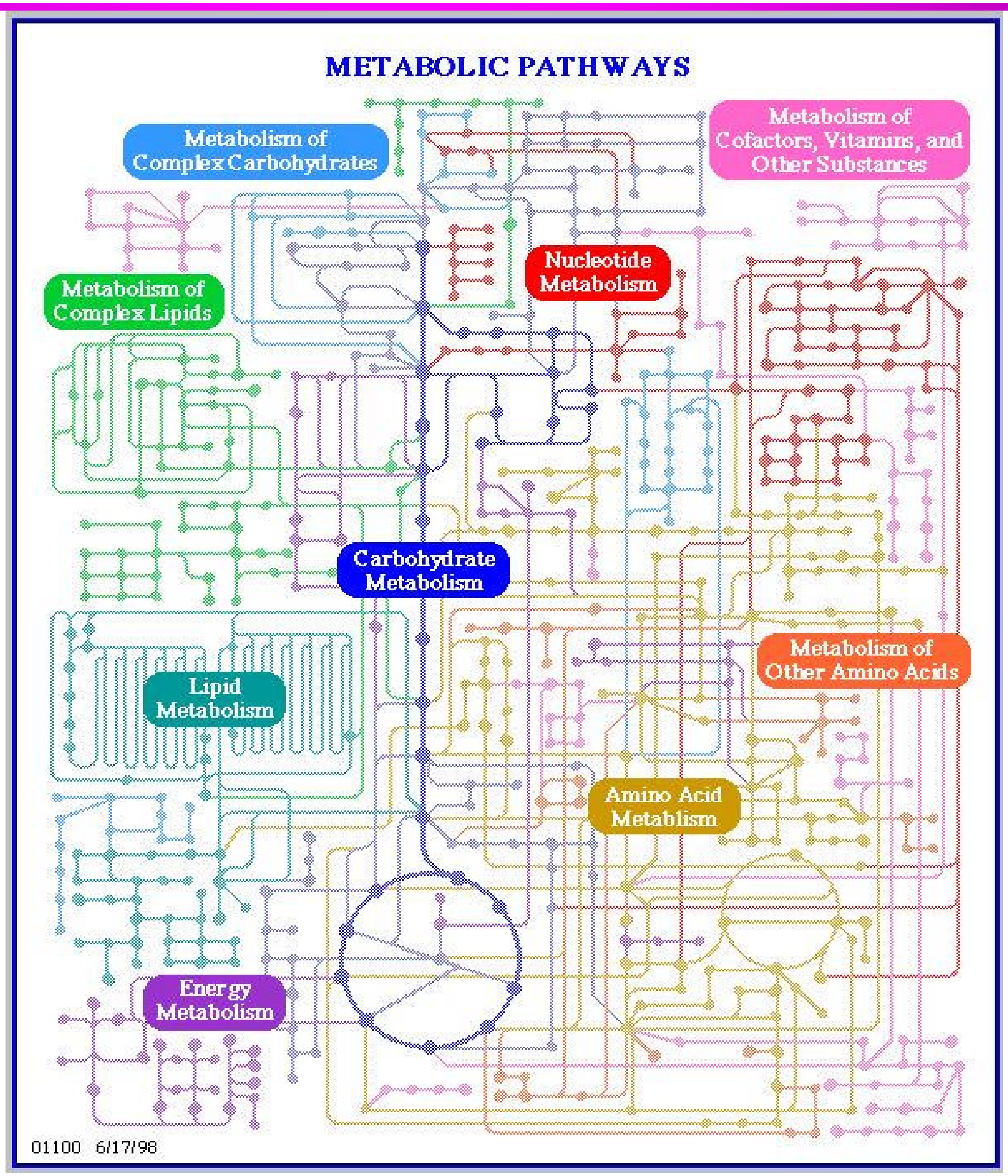
Models of Biological Systems

Just metabolism:

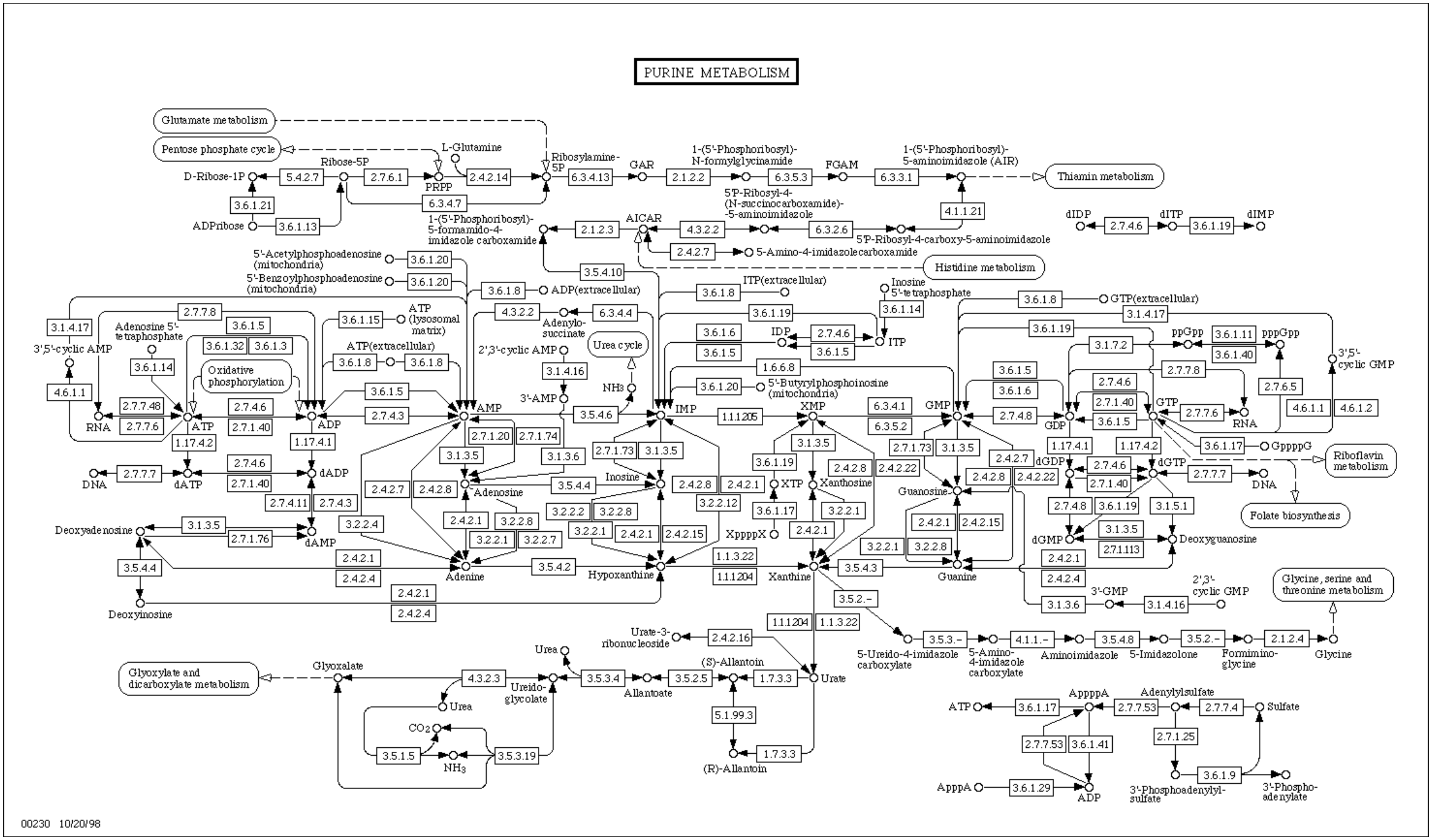
thousands of enzymes

thousands of reactants and products

reaction rates depend on concentrations of non-participants



One of ~80 such maps for metabolism:



Can we formulate and solve $dx/dt = f(x,t) + \text{flux}(t)$?

Not Yet

Unknown and poorly defined parts:

Human genes, a poorly characterized system:
Human has ~100,000 genes; We understand ~10,000.
(We just don't know all the pieces yet, But we have to start thinking about how we will take on these complex systems.)

Basic Metabolism, a well studied system:
Know the genes, but can only poorly measure their concentrations and in-vivo kinetics.

Know the reactants and products, but cannot measure their in-vivo concentrations.

3. SUMMARY & CONCLUSIONS

- Commercializing biology in the 21st century:
  - ➢requires integration of sciences, and engineering;
  - ➢Can we learn something from the past?
  - ➢analogy to “gold rush” (e.g. providing infrastructure for the “forty-niners”);
- Role of Engineers
  - ➢Wide variety of roles; mostly computational

ACKNOWLEDGEMENTS

- Bob LaROSSA (DuPont BCS & E):
- Bill FOSTER (DuPont Pharma)

Reprise: Solving Partial Differential Equations Using Excel 2000

by

Edward M. Rosen, EMR Technology Group

Introduction

The parabolic partial differential equation

$$\alpha * \partial^2 T/\partial x^2 = \partial T/\partial t \qquad (1)$$

with boundary conditions

At $t = 0$, $T = T_o$ at all x

At $t \geq 0$, $T = T_A$ at $x = 0$

and $\partial T/\partial x = 0$ at $x = L$

arises in the simulation of unsteady state heat conduction in a one-dimensional slab.

Initially the slab is at T_o. Then at $t \geq 0$, the surface ($x = 0$) is held at the constant temperature T_A. The other surface at $x = L$ is insulated.

In the above T is the temperature in K, t is the time in s and α is the thermal diffusivity in m^2/s. The parameters used are $T_o = 100$, $T_A = 0$ and $\alpha = 0.00002$.

The problem has been solved numerically by Cutlip and Shacham (1) using Polymath and the Method of Lines and by Taylor (2) using Maple and the Method of Lines. Subramanian and White (3) also used Maple to solve a similar problem but with a different boundary condition. It is the purpose of this study to compare the results of using Excel 2000 and finite differences with the results given in References (1) and (2).

Finite Difference Solution

The approach used here is that described by Rosen (4).

The temporal first derivative can be approximated by

$$\partial T/\partial t = (T_i^{k+1} - T_i^{k}) / \Delta t \qquad (2)$$

The second derivative can be approximated as (Crank-Nicolson method (5))

$$\partial^2 T/\partial x^2 = ½ *[(T_{i+1}^{k} – 2 T_{i}^{k} + T_{i-1}^{k})/ \Delta x^2 + (T_{I+1}^{k+1} –2 T_{i}^{k+1} T_{i-1}^{k+1})]/ \Delta x^2 \quad (3)$$

Letting

$$\Delta x = \Delta z * L \quad (4)$$

and then substituting Equations (2), (3) and (4) into Equation (1) and solving for T_i^{k+1} results in

$$T_i^{k+1} = (1/(\lambda+2) * [\lambda T_i^{k} + T_{i+1}^{k} – 2 T_i^{k} + T_{i-1}^{k} + T_{i+1}^{k+1} + T_{i-1}^{k+1}] \quad (5)$$

where

$$\lambda = 2 \Delta z^2 L^2/ (\alpha \Delta t) \quad (6)$$

In the above, subscript i is the space index and superscript k is the time index.

<u>Spreadsheet Implementation</u>

In order for the computation to be stable, the value of λ must be (Chapra et. al. (5))

$$\lambda \geq 4 \quad (7)$$

If Δt is chosen as 50 s and $\Delta z = 0.05$ (with L = 1) then $\lambda = 5$. The spreadsheet can then be set up with 21 columns of z (z = 0, 0.05, 0.10…. 1.00) and with rows starting with t = 0 with increments of 50 s.

Each cell in the first row is set up to be equal to T_o. All other cells (except z = 0. and z = L) are set up to be equal to T_o initially and then to implement Equation (5). Note that each cell utilizes the cells on each side of itself as well as the cells in the row above it.

The spreadsheet iterates until the values in each cell change only by a very small amount. Use is made of an IF statement in each cell to be able to test an initialization parameter to see if the cell should be set to the initial value or to be calculated by Equation (5).

The cells at z = 0 in each row are set to T_A. The cells at z = L utilize the the first derivative form (Chapra et. al (5))

$$\partial T/\partial x = (3 T_i - 4 T_{i-1} + T_{i-2})/ 2 \Delta x \quad (8)$$

Since this must be zero, the value of T in the cells at z = L (at all times) becomes

$$T_i^{k+1} = (4 T_{i-1}^{k+1} - T_{i-2}^{k+1})/ 3 \quad (9)$$

Results and Conclusions

Figure 1 is an excerpt from the final spreadsheet (after all the iterations were completed). The values of the temperature at time = 6000 s (not shown in Figure1) are shown in Table 1 and compared with the results in References (1) and (2).

z	Reference 1 $\Delta z = 0.05$	Reference 2 $\Delta z = 0.10$	This Work $\Delta z = 0.05$
0.	0.	0.	0
0.2	31.68	31.71	31.677
0.4	58.47	58.49	58.473
0.6	77.49	77.46	77.489
0.8	88.29	88.22	88.287
1.0	91.72	91.66	91.716

Table 1 Comparison of Temperatures at 6000s

The results compare well but it should be noted that Taylor used a space increment of 0.1 while Cutlip and Shacham and this work used 0.05.

Shacham and Cutlip (6) compare the use of different numerical programming packages (7) on a particular problem . In general, it appears that the selection of a particular package depends on the problem being solved, the familiarity of the user with that package, the particular package's strength and any cost that might be involved. (The author was quoted $1695 for Maple 6.1 as a standalone system). For this problem the use of Excel was straight-forward, did not require any training beyond the use of routine Excel (no VBA required) and involved no extra costs.

The complete spreadsheet may be downloaded from the author's website:
http://ourworld.cs.com/edwardmemrose

References

1. Cutlip, M. B. and M. Shacham, "The Numerical Method of Lines for Partial Differential Equations", *CACHE News*, Fall 1998, p 18

2. Taylor, R., "Engineering Computing with Maple: Solution of PDEs via the Method of Lines", *CACHE News*, No. 49 Fall 1999 p 5

3. Subramanian, V. R. and R. E. White, "Solving Differential Equations With Maple", *Chemical Engineering Education*, Vol 34 No 3 Fall 2000, p 328

4. Rosen, E. M. , "Excel 7.0: Partial Differential Equations", *CACHE News* No. 48, Spring 1999.

5. Chapra, S. C. and R. P. Canale, *Numerical Methods for Engineers*, McGraw-Hill, New York (1988)

6. Shacham, M. and M. B. Cutlip, "A Comparison of Six Numerical Software Packages for Educational Use in the Chemical Engineering Curriculum", Paper 2520 from American Society of Engineering Education Annual Conference, Seattle, Wash. June 28-July 1, 1998

7. Phillips, J. E. and J. E. DeCicco, "Choose the Right Mathematical Software", *Chemical Engineering Progress*, July 1999, p 69.

Heat Conduction In a One Dimensional Slab
Unsteady State- CACHE News Fall 1998

Initial	0		
Alpha	0.00002	Lambda	5
To	100		
TA	0		
L	1		
Del z	0.05		
Del t	50		

Index	Time (sec)	0	0.05	0.1	0.15	0.2	0.25	0.3	0.35
1	0	0	100	100	100	100	100	100	100
2	50	0	70.82039	95.74275	99.37888	99.90938	99.98678	99.99807	99.99972
3	100	0	56.50161	87.30734	97.22225	99.45964	99.90145	99.98275	99.99706
4	150	0	48.06492	79.64224	93.78491	98.41842	99.64142	99.92475	99.98505
5	200	0	42.44938	73.30869	89.93489	96.8201	99.12423	99.7821	99.94974
6	250	0	38.39662	68.11952	86.1297	94.85494	98.33545	99.51831	99.87246
7	300	0	35.30428	63.82057	82.55485	92.69978	97.31362	99.11596	99.73527
8	350	0	32.84837	60.20517	79.26696	90.47868	96.11603	98.57693	99.52568

Figure 1   Excerpt from Final Spreadsheet

GAMS Newsletter Number 3

by Bruce McCarl

GAMS Library expanded

GAMS using the new Library Manager discussed in the last newsletter and some internal developments has expanded the model library. Among other things, the new models illustrate use of some of new solver and GAMS capabilities (such as the use of constrained nonlinear system CNS: models as illustrated by korcns,gancnsx,gancns,camcns, as well as the use of MINLP models with integers:spring,pump,trimloss,gear) and some modeling tricks (ways to include discontinuous functions like abs, min, max, and sign using discrete variables as illustrated in absmip, and the importance of initial starting points in NLP models: circle). A complete list of the model library files including the new ones is on http://www.gams.com/modlib/modlib.htm.

Developments Regarding Solvers

GAMS continuously works on and updates the software it releases. Recent releases particularly the most recent (19.6) embody some developments on the solver front

Namely

1. CPLEX 7 is available and features a simplified licensing process plus improved (more compact) memory management for the branch and bound tree.

2. XPRESS is another choice for large LP and MIP problems and now runs on many platforms.

3. There is a new solver for solving MINLPs: SBB. An announcement on its capabilities and procedure to obtain an evaluation license are on http://www.conopt.com/sbb/SBB_announcement.htm A manual on it is in http://www.gams.com/docs/solver/sbb.pdf.

4. DICOPT can now solve models with integer variables even though the documentation says 0-1 only

The BDMLP solver which is included when you buy base GAMS now can solve mixed integer problems. Note however that this is not a highly capable solver and the other choices such as CPLEX, OSL, XPRESS, XA are generally better for extensive MIP work.

For more solver details see http://www.gams.com/solvers/solvers.htm.

Courses offered

I teach advanced GAMS in Texas in January 2001. Further information and other courses are listed on http://www.gams.com/courses.htm.

Conditional Compilation

Do you know that there is a command language in GAMS that permits substitutable parameters and you can write code that for example deals with a set if a set is sent to it or a parameter when it receives a parameter. For details see http://www.gams.com/mccarl/control.pdf

Change Options from Command line

You can specify many of the GAMS options by adding to the command line
(or the command line box in the IDE)

```
gams copper mip=xpress limrow=10 optcr=0.01
```

Presentations and Additional Documentation

GAMS has introduced a new section on it's web server which features GAMS related presentations at http:/www.gams.com/presentations/. Among others you find nine presentations from the Fall 2000 INFORMS meeting and my collection of GAMS documents.

This newsletter is not a product of GAMS Corporation although it is distributed with their cooperation.

November 20, 2000

Industrial Supporters of CACHE

We would like to thank the following companies for their generous support of the CACHE Corporation in 2000

AEA/Hyprotech

Air Products and Chemicals, Inc.

Aspen Technology

DuPont

Eastman Chemical Company

Exxon/Mobil

Equilon

Institute Mexicano del Petroleo

Merck & Company Inc.

Pfizer/Parke Davis

Union Carbide Corporation

Chemical Engineering Departments
Supporting CACHE

CACHE annually solicites universities for funds to carry out on-going CACHE activities and nurture new projects. The following is a list of our generous supporters

Ben-Gurion University, Israel
Brigham Young University
Bucknell University
California Institute of Technology
California State Polytechnic Univ, Pomona
Carnegie-Mellon University
Case Western Reserve University
Christian Brothers University
Chulalongkorn University
City College of New York
Clarkson University
Clemson University
Cleveland State University
Colorado School of Mines
Colorado State University
Cork Institute of Technology
Cornell University
Curtin University of Technology
Dalhousie University, Canada
Darmstadt University of Technology
Drexel University
Ecole Polytechnique
Florida Institute of Technology
Fundacao de Ensino e Engenharia de Santa
Georgia Institute of Technology
Groningen University
Helsinki University of Technology
Hong Kong University of Science & Tech.
Illinois Institute of Technology
Imperial College
Indian Institute of Technology, Bombay
Indian Institute of Technology, Kanpur
Institut fur Verfahrenstechnik, ETH
Iowa State University of Science and Technology
KAIST
Kansas State University
Kasetsart University
King Mongkut's Inst. of Tech. Thonburi
Konkuk University
Lafayette College
Lakehead University
Lamar University
Lehigh University
Louisiana Tech University
Manhattan College
McMaster University
McNeese State University
Michigan State University
Michigan Technological University
Mississippi State University
New Jersey Institute of Technology
New Mexico State University
North Carolina Agricultural & Technical State University
North Carolina State University of Raleigh
Northwestern University
Norwegian Institute of Technology
Ohio State University
Ohio University
Oklahoma State University
Oregon State University
Pennsylvania State University
Polytechnic University, NY
Princeton University
Purdue University
Queen’s University
Rensselaer Polytechnic Institute
Rice University
Rose-Hulman Institute of Technology
Rowan College
Royal Military College of Canada
Rutgers State University
South Dakota School of Mines & Technology
State University of New York at Buffalo
Stevens Institute of Technology
Swiss Federal Institute of Technology (EPFL)
Syracuse University
Technion-Israel Institute of Technology
Texas A&M University
Tri-State University
Tufts University
Tulane University
Tuskegee University
Universidad de Concepcion
Universidad Nacional de la Plata
Universidad Nacional de Colombia

Loughborough University of Technology
Louisiana State University
Universidade do Minho

Chemical Engineering Departments Supporting CACHE

Universitat Autonoma de Barcelona
Universität Erlangen-Nürnberg
Universitat Kaiserslautern
Universitat Politenica de Catalunya
Universitat Rovira i Virgili
Université de Sherbrooke
University Autonoma Metropolitana
University College London
University of Adelaide
University of Alabama, Tuscaloosa
University of Alberta
University of Arizona
University of Akron
University of Bath
University of Bradford
University of Calgary
University of California, Davis
University of California, Santa Barbara
University of Cambridge
University of Cape Town
University of Cincinnati
University of Colorado
University of Dayton
University of Delaware
University of Florida
University of Houston
University of Idaho
University of Illinois, Urbana
University of Iowa
University of Kansas
University of Kentucky
University of Laval
University of Louisville Speed Scientific School
University of Maine
University of Maribor
University of Maryland, College Park
University of Massachusetts, Amherst
University of Massachusetts, Lowell
University of Michigan
University of Minnesota, Minneapolis
University of Minnesota, Duluth
University of Mississippi
University of Missouri, Rolla
University of Nevada, Reno
University of New Brunswick
University of New Hampshire
University of New Haven
University of New Mexico
University of New South Wales
University of North Dakota
University of Notre Dame
University of Oklahoma
University of Ottawa
University of Oulu
University of Pennsylvania
University of Pittsburgh
University of Queensland
University of Rhode Island
University of Rochester
University of Saskatchewan
University of South Alabama
University of South Carolina
University of South Florida
University of Southern California
University of Southwestern Louisiana
University of Texas at Austin
University of Tokyo
University of Toledo
University of Tulsa
University of Utah
University of Virginia
University of Washington
University of Wisconsin
University of Wyoming
Vanderbilt University
Villanova University
Virginia Polytechnic Institute
Wayne State University
Washington State University
Washington University
Widener University
West Virginia Institute of Technology
West Virginia University
Worcester Polytechnic Institute
Youngstown State University

CACHE
STANDARD ORDER FORM

CACHE Product Description	Qty.	Supporting	Non-Supporting	Total
AI Monograph - Volumes 1, 2, 3 & 4 (sold separately)		$20	$25	
AI Monograph Set (Volumes 1-4)		$50	$75	
CD-ROM - Volume 2 Student chapters and supporting departments Individual students and faculty Individuals with no academic connection		 $15 	 $20 $20 $50	
Chemical Engineering Problems with Solutions – CD ROM		$10	$10	
ChemSep Version 3.5 • without documentation • with documentation **(License agreement must be signed first)**		 $100 + annual $60 $135 + annual $60	 $115 + annual $75 $150 + annual $75	
Computers in Chemical Engineering Education		$15	$15	
EMR Technology Library		$25	$30	
KORF - Fluid Flow via Graphics **(License agreement must be signed first)**		$50 per yr.	$60 per yr.	
Interactive Computer Modules • per course • set of four		 $35 $100	 $75 $200	
MultiBatchDS Two (2) 3.5" PC disks Manual **(License agreement must be signed first)**		 $90 + annual $50 $10	 $120 + annual $75 $10	
Multimedia-Based Educational Applications of Computer Simulations of Chemical Engineering Processes (Dow, Amoco, Eastman, Mobil)		$200 per module plus annual $25	$200 per module plus annual $25	
Multimedia Education Laboratory Chemical Engineering Fundamentals in Biological Systems Material & Energy Balances Multimedia Modules Visual Encyclopedia of Chemical Engineering Equipment		 $25 $25 $25	 $25 $25 $25	
Open-Ended Problems in Chemical Reaction Engineering		$10	$15	
Polymath Version 5.0		$125 + annual $75	$150 + annual $100	
Process Design Case Study - Volume 1 Process Design Case Study - Volume 2 Process Design Case Study - Volume 3 Process Design Case Study - Volume 4 Process Design Case Study - Volume 5 Process Design Case Study - Volume 6 (with GAMS) Process Design Case Study – Volume 7 (binder & disk) OR (CD-ROM)		$15 $15 $15 $15 $20 $65 $40 $15	$35 $35 $35 $35 $40 $100 $80 $30	
Strategies for Creative Problem Solving • personal use only • domestic universities • overseas universities • industrial companies		 $65 $90 $90 	 $65 $90 $105 $210/machine	
TANKSPILL		FREE	FREE	
TARGET II **(License agreeement must be signed first)**		$5	$5	
THEN		$5	$5	
OTHER PRODUCTS (enter name and price if known):				
			TOTAL	

PREPAYMENT IS REQUIRED

Cost of international shipping is determined by destination and weight of order.

TO ORDER:

Please fill out information below and fax to:
(512) 295-4498

Payment (please check)

___ check (US funds, US bank)

___ Purchase Order

___ Credit Card

Mastercard or Visa ___________________________________

Card No: ____

Exp Date: ____

Exact Name on Card: __________________________________

Name: ____

Address: ____

____

____

Phone: ____

E-mail address: ____

Your signature: ____

Make checks payable to:

CACHE Corporation
P.O. Box 7939
Austin, TX 78713-7939

E-Mail: cache@uts.cc.utexas.edu **Fax:** (512) 295-4498 **Phone:** (512) 295-2708