

Computers in Chemical Engineering Education

BRICE CARNAHAN
Editor

CACHE

Computers in Chemical Engineering Education

Editor

Brice Carnahan

University of Michigan



CACHE
Austin

This monograph may be ordered directly from:

CACHE

P. O. Box 7939

Austin, TX 78713-7939

Telephone: (972) 775-2815

FAX: (972) 775-3051

Email: cache@uts.cc.utexas.edu

WWW: <http://www.cache.org>

©1996 by CACHE Corp.

All rights reserved.

ISBN: 0-9655891-0-2

LCCN: 0-96-072249

PREFACE

The first general-purpose electronic digital computer, the ENIAC, executed its first instruction in a laboratory at the University of Pennsylvania more than fifty years ago. From that seminal moment, the performance (choose almost any metric) of the digital computer and its impact on the life of the nation have grown year by year, virtually unchecked.

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 system interfaces and programming environments, supercomputers and parallel machines, vastly improved communication, the Internet, the World Wide Web, etc.), and continues to this day.

Clearly there is no end in sight. *Business Week* (October 1996) predicts that possibly in 1997, and certainly no later than 1998, the computing industry and its ancillary products and services (software, communications, etc.) will supplant the automobile industry and its ancillary products and services as the largest contributor to the US Gross Domestic Product. The only certainty is that the future, driven by the core technologies of computing and communication, will be a digital one, and that the centrality of “computing” in society, business, government, and yes, education, is assured.

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 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.

Starting about 1960, computing in chemical engineering education began its period of slow but steady growth. By the late 1960s, it was clear to many chemical engineering faculty

COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

that the computer could no longer be ignored because of (among others) the important role “computing” would play in the professional lives of chemical engineering graduates. In 1969, a few of the most computer-active faculty from several chemical engineering departments in the US and Canada formed CACHE (Computer Aids for Chemical Engineering Education) at a meeting in Ann Arbor. The mission of the new group was to promote both computer use in the chemical engineering curricula and cooperation (involving chemical engineering computing) among industry, academia, and government. CACHE has continued its original mission to the present, serving as a catalyst for introducing software and other instructional aids to chemical engineering faculty and students in both the US and abroad.

This monograph is an outgrowth of the 25th anniversary celebration for CACHE that included a Faculty Reception and an afternoon session at the November 1994 Meeting of the AIChE in San Francisco. Professors J. D. Seader (University of Utah) and Warren Seider (University of Pennsylvania), two founding members of CACHE, subsequently prepared an archival paper on CACHE activities and parallel developments in computing in chemical engineering education during the twenty-five year period 1969-94. I was asked by the CACHE Board to solicit other papers on computer-related topics from prominent chemical engineering faculty and to serve as editor of this monograph, *Computers in Chemical Engineering Education*. The twenty papers included cover a wide range of subjects, from the impact of computing in specific chemical engineering courses to more general topics, such as accreditation, multimedia instruction, numerical software, and laboratory automation. Most of the papers were written in 1995 and 1996 from the perspectives of past developments, present activities, and future directions.

I thank the thirty five authors of these papers for their outstanding contributions, and also for their patience with me in editing, compiling, and publishing this monograph. I also thank CACHE for distributing the monograph to individual chemical engineering departments and the AIChE Publications Office for including it as a bonus offering to academic and industrial libraries that subscribe to the AIChE Package Plan.

Brice Carnahan

CONTENTS

Role and Impact of Computers in Engineering Education.	1
Richard S. H. Mah and David M. Himmelblau	
Computing Skills in the Chemical Engineering Curriculum	9
Jeffrey C. Kantor and Thomas Edgar	
History of CACHE and its Evolution.	21
J. D. Seader and Warren D. Seider	
Interactive Computer-Aided Instruction.	57
Susan Montgomery and H. Scott Fogler	
General-Purpose Software for Equation Solving and Modeling of Data	73
Mordechai Shacham, Michael B. Cutlip and N. Brauner	
Thermodynamics and Property Data Bases	85
Aage Fredenslund, Georgios M. Kontogeorgis and Rafiqul Gani	
CACHE's Role in Computing in Chemical Reaction Engineering	103
H. Scott Fogler	
Transport Phenomena.	125
Bruce A. Finlayson and Andrew N. Hrymak	
Separations Processes.	139
Ross Taylor	
Conceptual Design and Process Synthesis	153
James M. Douglas and Jeffrey J. Siirola	
Process Simulation	161
Lorenz T. Biegler, J. D. Seader and Warren D. Seider	
Optimization	171
Ignacio E. Grossman	

COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

Design Case Studies	185
Ignacio Grossmann and Manfred Morari	
Process Control.	193
Yaman Arkun and Carlos E. Garcia	
Laboratory Automation and Real-Time Computing.	203
Duncan A. Mellichamp and Babu Joseph	
CACHE and the Use of Computer Networks for Education	211
Peter R. Rony	
Intelligent Systems in Process Operations, Design and Safety.	227
Steven R. McVey, James F. Davis and Venkat Venkatasubramanian	
Languages and Programming Paradigms	239
George Stephanopoulos and Chonghun Han	
Visualization.	253
Andrew N. Hrymak and Patricia Monger	
2001.	265
Brice Carnahan	
Author Index.	281
Subject Index	283

ROLE AND IMPACT OF COMPUTERS IN ENGINEERING EDUCATION

Richard S. H. Mah
Northwestern University
Evanston, Illinois

David M. Himmelblau
University of Texas
Austin, Texas

Abstract

After three and half decades of development, the computing environment is now highly interconnected. Networks proliferate between computers, laboratories, buildings, campuses and across continents. Use of computers is integrated with many chemical engineering courses in teaching, learning, and communication. Many pioneers' dreams are already a reality. With computers, one can cover more course material using more realistic illustrations.

The continuing decline in the computer price/performance ratio makes it affordable to create software which is not just functional, but also fault-tolerant and user-friendly, making it useful and accessible to a wide community of users who have limited or no formal training in computers. Enhanced capabilities of general purpose software, like Matlab, diminish the need for chemical engineers to program in Fortran and other procedural languages. With ever-improving software the bottleneck on process analysis rests once again on the quality and fidelity of the model, and we are back to the basics.

One important impact of computers on engineering education is to broaden the access to teaching and learning styles. New pedagogy creates opportunities for curriculum re-vamping which will surely be needed at some point, since we cannot go on adding new material to the existing courses without deleting other topics. By broadening our choices in pedagogy we may also make our profession more accessible to a wider range of candidates.

Historically, the path to progress is strewn with expensive wreckage. Megabuck investment does not ensure that a project will succeed, and today's success is no guarantee for tomorrow. But there is no sign that the pace of development in computing and information technology is slowing down. How engineering education can continue to make use of these rapid changes remains a challenge. An education built on sound fundamentals and in-depth understanding is the best strategy to allow one's knowledge base to evolve and grow with changing times. While hands-on practical experience is indispensable to engineers, one must avoid over-specialization. Kilobit education is dangerous in a world of gigabyte technology.

On the other hand, history also shows that the momentum generated by a real winner can go a long way. Fortran, LP, word processors, and E-mail are some examples. We

now have a global market for buyers and sellers of information technology, vast capital and financial institutions, vast trained manpower, and many potential winners. A list of promising developments include networks, optical and parallel computers, CD ROMs, satellite broadcasting and reception, personalized portable phones and pagers, notebook computers, and high definition television. There is a great likelihood for information technology mergers, and high potential that such mergers will create new products and technology which will further enhance the use of computers in engineering education.

We are almost at the dawn of the 21st Century. Looking back along the pathway leading to the present, we realize how far we have traveled in a journey propelled by the success of a few key inventions, and how many more wonders lie ahead of us to be discovered, invented and applied to engineering education in the decades ahead. The prospect is truly exhilarating and exciting.

Current Status

The Computing Environment

When the university is in session, the chances are that the lights are on, the computers are running in the Computer Teaching Lab, and students are using the computers in various ways, some of which their older brothers or sisters, just a few years ago, could not have done. The Computer Teaching Lab is now easily the most used facility in the chemical engineering department. System crash is now a rare event. The opening hours are only dictated by security and maintenance considerations. There is no full time staff associated with this facility. It is user-serviced with a half-time teaching assistant acting as the Lab Manager. Only policy guidance and planning are provided by a faculty director. Fourteen hours a day during the week and eight hours on Saturday and on Sunday the micros slave tirelessly at the friendly commands of users. The micros are connected in a local area network (LAN), served by a file server, printers and other peripherals. The LAN is linked to the campus fiber optic backbone, and through it, to the Internet worldwide.¹

Access to information superhighway is the most significant step forward in the empowerment of faculty and students, which has taken place on many campuses, while the process continues in others. Give and take a few details such as types of hardware and software, the physical dimensions of the lab, and the size of the student population, the environment described above is the computing and information processing environment currently existing in many universities, and the computing facilities available for chemical engineering education.

Impact of Computers on Chemical Engineering Education

We are concerned here with engineering education, with specifics taken primarily from chemical engineering. How have computers affected the learning and teaching of engineering? To continue with our example, the use of computers is now closely integrated in most of our current undergraduate courses, beginning with material balances and stoichiometry (analysis of chemical process systems), thermodynamics, equilibrium separations, continuing with pro-

¹. In this simplified description we omitted a few hardware and software details, which are transparent to the user.

cess dynamics and control, process design, process optimization, and chemical engineering lab, and ending with electives such as statistics in process modeling. Significant changes have already taken place in content, learning and the teaching of these subjects. For instance, linearization and Laplace transformation play a ubiquitous role in classical process control. In the days before computers were available, much time was spent on inverse transformations, and the preparation of Bode and Nyquist diagrams in stability analysis. Now, with Program CC, we simply input the appropriate polynomials in the numerator and denominator of the transfer function in the Laplace domain, and let the computer, the program, and the graphics do the tedious work. Parametric studies are easy to carry out. Understanding and insight, which used to take a long time to develop, are now acquired rapidly and enthusiastically. Similarly, TK-solver and Lotus 1-2-3 take a lot of drudgery and mystery out of balances and stoichiometry. With flowsheet simulators and property libraries, the dual role of thermodynamics in process analysis and in property estimation becomes very much easier to teach and explain. In statistics, by using Monte Carlo simulation, the instructor can readily demonstrate and verify, for instance, the Central Limit Theorem, and display plots in vivid color graphics in dimensions which "will cross a rabbi's eyes" ("Fiddler on the roof").

The upshot is that by using computers one can cover more territory and tackle more realistic problems with less time and more fun. With the availability of these new tools and techniques, it is possible to begin experimenting with new pedagogy (Felder and Silverman 1988, Schank 1994, and Stice 1987), which, in time, may profoundly change the ways students learn and instructors teach these subjects. This is particularly true with subjects involving many elements, complex structures and closely knit relationship, such as systems engineering, which would be difficult to demonstrate experimentally. With computer simulation we can reproduce precisely controlled "misbehavior" to study its impact on every aspect of the system.

Communication and Productivity Tools

Equally remarkable are advances which have taken place in communication and personal productivity tools. Students are expected to acquire serviceable skills in word processing, graphics, desktop publishing, database and E-mail with only a modicum of formal instructions. With Spell Check there is no excuse not to get the spelling right.

By making it fun to prepare texts and illustrations, not only do the reports and illustrations begin to look more professional, but the substance and style also improve in due course. With universal access to computer networks, everyone can send a message or be reached via E-mail without having to play phone tag. Through remote access the instructor could just as easily review class records and assign homework problems as he or she could conduct an electronic dialog with a colleague at another location - all without leaving the physical environment of home or office. Last but not least, by greatly simplifying the protocol, distribution and delivery, the E-mail lowers the threshold of communication and shrinks the physical and psychological distances of an organization, be it a corporation, a government or an university.

To appreciate that profound and pervasive changes are rapidly taking place in information technology in general, and computers in particular, we need only look back to the path of progress, which has led us to the present state of development.

Highlights of the Past

By most reckonings we are in the fourth decade of computer applications, even though there may not be an exact point of origin. The first two decades were dominated by mainframes and minis. In chemical engineering much of the initial programming efforts were directed at replacing repetitive calculations. Taking 1958 as our reference point, the establishment of Fortran as the universal high level programming language for quantitative computation must rank among the foremost achievement of the first decade. By the second decade, LP and more specifically, codes based on the Simplex Method, had become the single largest user of computer time in the process industries. Time sharing, on-line terminals, and flowsheeting programs were some of the other notable developments of that decade. The year 1978 heralded the introduction of the first commercial scale microcomputers, the Apple II, followed three years later by the IBM PC and the mass marketing of software: word processor, spreadsheet, and database, which fueled the revolution of microcomputers. By 1990 personal computers (PCs, clones, Apples and Macintoshes) became widely owned, second only to telephones in number of units sold (Carnahan and Likes, 1993). It is notable that E-mail and networking did not gain popularity until well into the third decade.

One of the most remarkable characteristics of the computer industry is the continual improvement in performance in relation to price, which has been sustained for over three decades already. Figure 1 and Figure 2 show that the price of computing has dropped by one-half every 2 to 3 years ever since computers were marketed commercially. A \$3,000 PC now is comparable in computing speed to a million dollar mainframe a decade ago. If progress in the rest of the economy had matched progress in the computer sector, a Cadillac would cost \$4.98, while 10 minutes' worth of labor would buy a year's worth of groceries (Brynjolfsson, 1993).

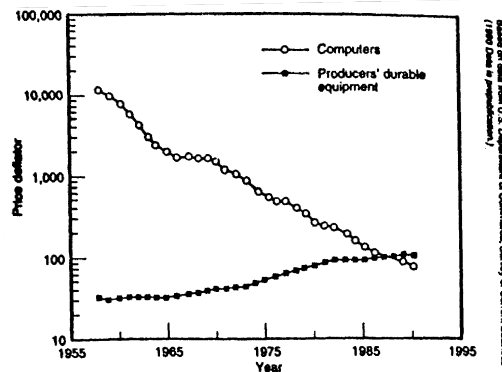


Figure 1. The cost of computing has declined substantially relative to other capital purchases.

What Has Already Happened or is Happening

One impact of the changing price/performance ratio is improved user-friendliness. In early 1980s a word processor ran on a 64 KB memory microcomputer. By the mid 1980s it requires 640 KB of memory. In 1994 no respectable application software requires less than

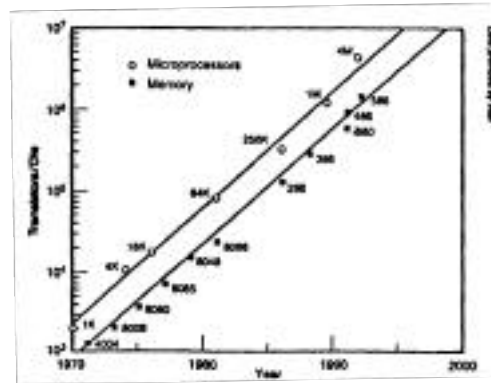


Figure 2. Microchip performance has shown uninterrupted exponential growth.

several megabytes of memory. However, with this extravagance in memory requirements came a much more fault-tolerant and user-friendly interface, and the same “look and feel” (under Windows, for instance) which make the task of assimilation much less formidable for lay users. In fact, previous emphasis on learning to program in Fortran and similar high level languages has diminished, as Matlab, MathCad, Polymath, Mathematica and their ilk enhance their capabilities, and relieve users of the requirement to program, raising anew the question whether there is a need to teach programming except to computer engineering and computer science majors.

With ever-improving computing capabilities and methods of solution, the bottleneck in process analysis is once again the quality and fidelity of the models suitable for different applications. Some attention is already being directed to applications typically ignored by educators, such as modeling less structured, fuzzy problems, and applications involving noisy and correlated data.

Cheap information storage and improved means of transmission and distribution have already changed the modus operandi of traditional institutions such as libraries and publishing houses. Journal abstracts and even articles are sold on compact disks which can be searched at will at nominal costs, and with an E-mail address and access to databases a student can download information just as easily as he can send an electronic file to a friend. Textbooks have changed substantially. Readers are expected to have access to a computer to solve exercise problems. Disks containing pertinent software are commonly found in inserts in the back of books. The technology exists today to customize, assemble, and electronically deliver textbooks for each student. But it may take time to resolve all the copyright issues and to provide suitable marketing mechanisms. How to provide teaching material for engineering courses will almost certainly be a major issue in the next decade, and the opportunities for innovation will be limited only by our imagination.

One important impact of computers on engineering education is to broaden the access to teaching and learning styles. In a few instances, computer-aided learning has completely replaced the lecture-recitation format for learning. But in most universities, changes have oc-

curred in a more limited way over a period of many years, as the role of computers in education became better appreciated by the faculty. Such changes that have taken place are often caused more by the influx of young faculty members who have hands-on knowledge in using computers than by the action of accreditation or university guidelines. So retooling of tenured faculty may well be one limiting factor in introducing new information technology in our pedagogy. Nonetheless, the rate of technological innovation will continue to be rapid, and equipment will be technologically obsolete when it is still in good mechanical conditions. Short life cycles in computing technology will continue to be a fact of life. To stay in the competition, schools must have plans and funding to rejuvenate programs and facilities. Those with a foresight to anticipate will have a competitive advantage.

Curriculum revamping will surely be needed at some point, since we cannot go on adding new material to the existing courses without deleting some other topics. This will create opportunities for experimenting with new pedagogy, which may in turn make our profession more accessible to a wider range of candidates, thereby contributing to the national workforce retooling.

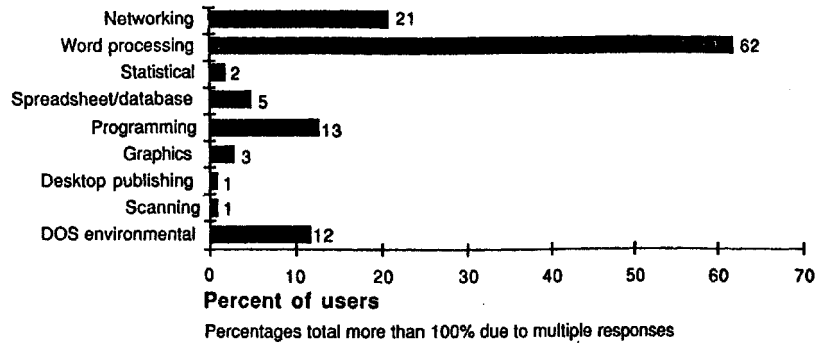
Historically, the path to progress is strewn with expensive wreckage. Megabuck investment does not ensure that a project will succeed, and today's success is no guarantee for tomorrow. An example of innovative educational software is the PLATO system, which reportedly cost CDC hundreds of millions of dollars in the 1970s, but which has left no lasting imprint on engineering education today. However, we did learn some valuable lessons. Most potential users cannot visualize how to use unfamiliar technology in large mental steps. If the context of the new technology is sufficiently dissimilar to the current context, rejection is likely. Thus, quantum leaps often fail where incremental changes may succeed. Another lesson for developers of new computing technology is to focus on the relevance to the educational needs and not be carried away by the clever, exciting or imaginative technology. Changing curriculum solely to take advantage of computing technology is usually a waste of resources.

The Future

There is no sign that the pace of development in computing and information technology is slowing down. An education built on sound fundamentals and in-depth understanding is the best strategy to allow one's knowledge base to evolve and grow with changing times. While hands-on practical experience is indispensable to engineers, one must avoid over-specialization. Paraphrased in another way, kilobit education is dangerous in a world of gigabyte technology.

On the other hand, history also shows that the momentum generated by a real winner can carry development a long way. Fortran, LP, word processor, and E-mail are some examples. Word processing was probably the single largest application which spearheaded the commercialization of personal computers. Figure 3 (Alspach, 1993) shows that it continues to be the dominant application of microcomputer users even today.

Compared with the earlier decades when IBM accounted for 3 of every 4 computers sold, we now have a global market for buyers and sellers of information technology, vast capital and financial institutions, vast trained manpower, and many potential winners. A list of promising



Graphic by Steve Alspach

Figure 3. Types of software and usage in computer laboratories.

developments include networks, optical and parallel computers, CD ROMs, satellite broadcasting and reception, personalized portable phones and pagers, notebook computers, and high definition television. The potential for information technology mergers which will further enhance the use of computers in engineering education is very large and very likely.²

We are almost at the dawn of the 21st Century. Looking back along the pathway leading to the present, we realize how far we have traveled in a journey propelled by just a few key inventions, and how many more wonders lie ahead of us to be discovered, invented and applied to engineering education in the decades ahead. The prospect is truly exhilarating and exciting.

References

- Alspach, S. (1993). News and Views, vol 2, No. 3/Spring 1993, NU information Systems and Technology, Northwestern University, Evanston, Illinois.
- Augustine, N.R. (1994). Socioengineering Age. ASEE Prism, 24-26, February.
- Brynjolfsson, E. (1993). The productivity paradox of information technology. Comm. ACM, Vol. 36, No. 12, 67-77, December 1993.
- Carnahan, B., and J.O. Wilkes (1994), The IBM PS/2, OS/2, and The Michigan Computing Environment. College of Engineering, The University of Michigan, Ann Arbor, Michigan.
- Felder, R.M., and L.K. Silverman (1988). Learning and teaching styles in engineering education. Engineering Education. 674-681, April, 1988.
- Schank, Roger (1994). How Students Learn - Educational Software and the Future of Education. Sponsored by Searle Center for Teaching Excellence, April 21, 1994.
- Stice, J.E. (1987). Using Kolb's Learning cycles to improve student learning. Engineering Education. 291-296, February, 1987.

². Mergers are taking place even as we write. Novell and Word Perfect have just announced a new alliance to compete with Microsoft, which is teaming up with McCaw to form Teledesic, a global communication network linked by 840 satellites.