CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

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WHAT IS CACHE?

CACHE is a non-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 1960's, 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, 14 chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. Initially, the CACHE Committee was 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 on-going projects. Information on CACHE activities is regularly disseminated through **CACHE News**, which is published twice each year. Individual inquiries should be addressed to:

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CACHE NEWS

The **CACHE News** is published two times a year to report 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 D. M. Himmelblau with contributions from a number of CACHE members and representatives.

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STATUS OF FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

by J.D. Seader
University of Utah

As part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to departments of chemical engineering to install on their own in-house computers. Thus, departments would be able to run FLOWTRAN on their own computers at no charge other than that of their own computer center. CACHE is continuing the supervision of the preparation of FLOWTRAN load modules for a wide variety of main-frame, supermini, and supermicro-type digital computers and the distribution of the modules on magnetic tape to those departments that order them. Instructional books on FLOWTRAN are already available through CACHE by using the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

1. **DEC VAX 11-7XX** series of super minicomputers running with the VMS operating system.
2. **DEC 20XX** mainframe computer running with the FORTRAN-20, Version 7 compiler (9-track, 1600 BPI tape).
3. **UNIVAC 1100** series computers running under the EXEC 1100 (38R2/08) operating system with the FORTRAN 77-SID (10R/A) compiler (9-track, 1600 BPI tape).
4. **Amdahl** computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).
5. **IBM** and IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and 43XX with the following operating system and FORTRAN compiler combinations:

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	OS1/MVS	IV-H ext
c	OS/VS2 MVS	VS
d	CMS	IV-G1

6. **IBM PC-XT-370** personal computer operating in conjunction with an IBM mainframe.
7. **CDC Cyber** mainframe computers with the NOS operating system and a FORTRAN V compiler.
8. **Apollo Domain** work stations running with AEGIS operating system.
9. **Data General** MV super-minicomputers running with the AOS/VS operating system.

Conversions are also underway for the DEC 10, Honeywell, Sperry 90/80, DEC VAX under UNIX, and Prime machines. Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes but not for consulting. A total of 112 FLOWTRAN tapes have already been distributed to departments at the following universities for the computers indicated:

Amdahl 470:
Univ of British Columbia; West Virginia Inst of Tech; Univ of Ottawa

Amdahl 5860:
Univ of Michigan; Michigan State Univ

Amdahl V-8:
Wayne State Univ

Apollo DOMAIN:
Bucknell Univ; Univ of Michigan

CDC 6500:
Purdue Univ

CDC CYBER:
Oregon State Univ; Colorado State Univ; South Dakota School of Mines; Lehigh Univ; California State Poly Univ; Univ of Washington; Univ of Lowell

DEC 2060:
Case Western Reserve Univ; Columbia Univ; Worcester Polytech Inst

DEC VAX 11-730:
Aristotle Univ of Thessaloniki; Brown Univ

DEC VAX 11-750:
Univ of Arizona; Brigham Young Univ; Univ of Cincinnati; Colorado School of Mines; Florida State Univ; Georgia Inst of Tech; CUNY; Univ of Pennsylvania; Univ of South Florida; Univ of Southwestern Louisiana; Tuskegee Institute; Washington Univ; Univ of Washington; Widener Univ

DEC VAX 11-780:
Univ of Adelaide; Univ di Bologna; Univ of California, Davis; Univ of California, San Diego; Carnegie-Mellon Univ; Univ of Colorado; The Cooper Union; Univ of Delaware; Florida Inst of Tech; Grove City College; Univ of Houston; Illinois Inst of Tech; Iowa State Univ of Science and Tech; Laval Univ; Lowell Univ; Manhattan College; Univ of Massachusetts; McMaster Univ; Univ of Nebraska; New Jersey Inst of Tech; New Mexico State Univ; Univ of New South Wales; State Univ of New York at Buffalo; Northeastern Univ; Tech Univ of Nova Scotia; Pratt Inst; Rice Univ; Rose-Hulman Inst of Tech; Univ of Saskatchewan; Stevens Inst of Tech; Univ of Toronto; Univ Nacional del Sur; Univ de Concepción; Villanova Univ

DEC VAX 11-785:
Univ of Wisconsin

DG MV/8000:
Northeastern Univ

Honeywell DP39: Royal Military College of Canada

IBM 3033:
Rensselaer Polytech Inst; Texas Tech Univ; Howard Univ

IBM 3081:
Arizona State Univ; Clemson Univ; Drexel Univ; Louisiana State Univ; North Carolina State Univ, Raleigh; Univ di Pisa; Univ of Illinois, Chicago; Univ of California, Berkeley; Univ of Connecticut

IBM 3083:
Yale Univ

IBM 370:
Univ of Akron; Louisiana Tech Univ

IBM 4341:
Beijing Inst of Chem Tech; Cornell Univ; City Univ of New York; Ecole Polytech Univ of Montreal; Univ of Puerto Rico; San Jose State Univ; Univ of South Alabama; Syracuse Univ; Arizona State Univ

IBM 4381:
Inst Tech Estudios Superiores de Monterrey; Univ of Missouri-Rolla; Univ of Washington

IBM PC-XT/370:
Arizona State Univ

NAS 5000:
Univ de Sherbrooke

NAS 6630:
Kansas State Univ

NAS 6650:
Univ of Toledo

NAS AS:
Iowa State Univ of Science and Tech; Rutgers—The State Univ

Sperry 90/80:
New Jersey Inst of Tech

UNIVAC 1100:
Univ of Pennsylvania; Univ of Utah; Univ of Wisconsin; Kuwait Univ; Michigan Tech Univ; Mississippi State Univ

In order of popularity, the numbers of tapes distributed for the leading makes are:

DEC VAX: 51
IBM Mainframes: 27
CDC Mainframes: 8
UNIVAC Mainframes: 6

If you would like to obtain a FLOWTRAN tape for your computer and have not already expressed that desire to CACHE, complete and submit the form, FLOWTRAN TAPE, at the end of this newsletter. You will be required to sign a User's Agreement that must be approved by Monsanto. The cost of the tape, payable to CACHE, is $250. However, the charge to CACHE-supporting departments listed near the end of this newsletter is only $175.

Editorial Note: The following articles by Peter R. Rony were entered into the COMPMAIL+ electronic mail system, and transmitted directly to a UNIX typesetting system at the University of Texas without the need for retyping, editing, and proofing.

MICROCOMPUTER/PERSONAL COMPUTER NOTES

Edited by Peter R. Rony
Virginia Polytechnic Institute and State University

PART 1

Business Computer Systems (July 1985) reports the following fifteen "irrefutable laws of computer system operation" developed by Dr. Michael Kasavana, Professor of Computer Science at Michigan State University School of Hotel, Restaurant, and Institutional Management.

1. Any computer program that runs well is obsolete.

2. A good computer program is always accompanied by extremely bad documentation.

3. The value of a computer program is inversely related to the weight of its output.

4. Program complexities always grow to exceed the capabilities of the programmer responsible for it.

5. Any time a system appears to be working well, something has been overlooked.

6. What you don't do is always more important than what you do.

7. In any computer program, constants should always be treated as variables.

8. Investments in system-reliability products always exceed the probable cost of errors they are designed to avoid.

9. The problem is not that computer salespeople are not knowledgeable, it's that most of what they know isn't true.

10. If a system requires "n" number of spare parts, there will always be "n-1" parts in stock.

11. Major software revisions are always requested after software installation is completed.

12. Installation and operating instructions are always discarded with the shipping containers.

13. Any component part requiring the most frequent service or adjustment will be the least accessible.

14. Undetectable errors are infinite while detectable errors, by definition, are finite.

15. Nothing is impossible for the person who doesn't have to do the work.

The Amiga Personal Computer, a 68000-based machine manufactured by Commodore International, is described in the August 1985 issue of **Byte**. For a list price of $1295, you get a 7.15909 MHz 68000; 256K bytes dynamic RAM, user expandable to 512K bytes (machine's design allows for a maximum of 8.5 Megabytes); 192K bytes of ROM containing multitasking, graphics, sound, and animation support routines; five modes of graphics, including 640 by 400, 16 colors; built-in 3.5-inch double-sided disk drive for disks that hold 880K bytes in 160 tracks; detached 89-key keyboard with calculator pad, function, and cursor keys; disk port onto which three additional disk drives can be connected in daisy chain fashion; serial port with maximum transfer rate of 500,000 bits/second; Centronics-compatible parallel port; bundled software that includes AmigaDOS and ABasiC; two stereo audio jacks; RGB analog, RGB digital, and NTSC composite output. This machine should put price pressure on the Apple Mac.

Declarative languages are also featured in the August 1985 issue of **Byte**. Article titles include "Prolog Goes to Work," "Logic Programming," "Declarative Languages: An Overview," "Program Transformation," "Functional Programming Using FP," and "A HOPE Tutorial." What is a declarative language? To quote Susan Eisenbach: "The major goals of declarative programming are to provide structurally transparent languages, so programs can be verified and optimized mechanistically, and to facilitate the implementation of multiple-instruction, multiple-data parallelism in the coming generation of parallel-processing computers. The way that declarative languages attempt to achieve these goals is by separating the task that the program is to perform from the way that the computer is to do it. That is, unlike imperative programming languages, declarative languages do not specify the flow of control but only the flow of data in a program." Interesting reading.

"New Microprocessor Chips" are briefly discussed by Philip Robinson in **Byte** (August 1985, page 369): iAPX 386, 80C86, and the AT Probe. "The iAPX 386 (the official name for the 80386) is made using CHMOS III technology. CHMOS is Intel's latest version of the CMOS process. The 386 is pipelined, has a high-bandwidth 32-bit bus, and supports full 32-bit addressing (4 gigabytes of physical space, 4 gigabytes per segment, and 64 terabytes of virtual address space per task). The 386 also has memory management and protection (compatible with the 286), virtual-memory support, caches, and paging (optional) all on chip. It can handle 8-, 16-, and 32-bit data, has a multiple-coprocessor interface, and supports integrated multitasking. The 386 is object-code software-compatible with the 8086, 8088, 80186, 80188, and 80286. The 386 instruction set is a superset of the 286 set. All instructions are extended to support the 32-bit addresses and operands. . . That means 8088 programs (such as those for the IBM PC) should run without recompilation on an 80386 box." It appears that Intel will continue to be in the driver's seat in its competition with the Motorola 68000 family of microprocessors. Industry standardization around the IBM PC line should continue without serious challenge for the next several years.

Georg Raeder, in "A Survey of Current Graphical Programming Techniques" (**Computer**, August 1985), provides succinct commentary on alternative graphical programming techniques. Examples: (a) "Flowcharts were originally developed as tools for assembly language programming. They clarify a program's control structure, but do not describe its data structure." (b) "Nassi-Schneiderman diagrams impose structure on program control; however, they do not display expressions, procedure calls, types, and data graphically." (c) "State diagrams lack support for data and control structures and can be used only for simple, automoton-type program pieces, but they illustrate very clearly how those pieces parse input and generate output." (d) "Petri nets are often used for hardware descriptions. They use a token mechanism to show control flow." (e) "Dataflow diagrams have been used mostly in connection with dataflow languages and systems." He comments on recent graphical-programming systems such as the Program Visualization environment, Omega, PegaSys, Pecan, and Programming-in-Pictures.

The August 1985 issue of **Dr. Dobb's Journal** provides what they believe is the definitive C compiler review in "C Compilers for MSDOS," by the PicoNet C-SIG and the SVCS. "These two groups have assembled a suite of 30 benchmarks, run them through the most popular MSDOS compilers and interpreters, and tabulated the results." If pressed to declare a winner, the authors would probably select the Microsoft or Aztec compilers. The Wizard compiler had excellent diagnostics, and the Mark Williams compiler had the best debugger.

Electronics Week, a McGraw-Hill publication, has reverted back to its old name, **Electronics**. The July 1, 1985 issue has several articles of interest: (a) "Dual

Operating Systems: A Compromise in Quest for a Standard," (b) "Will 'Smart House' Provide Shelter for High-Tech Firms?," and (c) "The Pell-Mell Rush Into Expert Systems Forces Integration Issue." Replacing the common two-plug 110-Volt AC receptacle in the U.S. is a proposed smart-house wiring scheme that integrates electricity, telephones, security, and fire detection while distributing audio, video, and data throughout the home. A picture of the new receptacle is shown on page 45. Now, if somebody could figure out how to retrofit millions of homes and buildings with such a receptacle as well as good reasons why one should do so, a revolution in home communications could be launched. Concerning article (c), "It is likely that nearly every major U.S. corporation has or is initiating an AI group to start building—or at least start looking at—expert systems." The teaching of principles of AI and expert systems will become very important, if not fashionable, in engineering colleges during the next several years.

This column is being typed on a dual operating system system, namely, the Zenith Z-100, which has both CP/M-85 and ZDOS (a dialect of MSDOS). The author also has access to a university-owned IBM PC. What are the advantages and disadvantages of owning a Z-100 relative to an IBM PC? Perhaps the biggest disadvantage is the fact that S-100 bus add-on boards for the Z-100 are considerably more expensive than their IBM PC bus counterparts. Software has proven to be less of a problem, in general, because many of the most popular software packages operate on either machine. For example, PeachText 5000, Microsoft FORTRAN, and Turbo Pascal can be configured for either machine. Media Master, a disk-to-disk format conversion software package, makes text files on IBM PC diskettes accessible to the Z-100.

COMPAQ must be doing very well in the depressed computer market. The author encountered 7-page, glossy, color ads in a variety of magazines in recent months. COMPAQ focuses only on the business market. The COMPAQ DESKPRO 286 is an IBM PC/AT clone, but has several improved features.

PART 2

Megacells (a form of standard cell) and application-specific integrated circuits (ASIC): two very important recent developments in VLSI semiconductor technology. Both topics are discussed in **Electronics** (July 15, pp. 56-58, and July 22, pp. 40-45). Integrated circuit technology has moved up one architectural level. Now, circuits that used to be sold as individual microprocessors or programmable interface chips (e.g., 8250, 8254, 8255, 8259, 8237, 6845, ROM, 6502, and so forth) are being combined as standard cells to permit rapid integration of systems and subsystems—disk controllers, counters, serial and parallel I/O, and microprocessors—within a single chip. Megacells now or soon available from VLSI Technology Inc. include CMOS-based functions such as the 82C54, 82C84, 68C45, 65C02, 82C50, 82C59, 82C55, 82C88, and 82C37A. An entire CPU board (with the exception of RAM), perhaps a group of boards, will be shrunk within the next several years into a single, large integrated circuit with 40 to 128 pins. The importance of standardization in such efforts cannot be overemphasized. Standard microprocessor instruction sets and standard programmable functions will be used, thus preserving software skills of microcomputer system designers that date back to the mid-1970s, when programmable interface chips were first introduced by Motorola and Intel. Note also the trend to CMOS technology.

Continuing our discussion of application-specific integrated circuits (ASIC), standard cells, macrocells, megacells, and supercells, Figure 4 in the July 22 issue of **Electronics** (page 43) shows a single CMOS silicon chip created at Zymos that contains 87 of the 90 ICs that comprise the IBM Personal Computer AT motherboard. The chip holds the equivalent of 25,000 gates. A PC-on-a-chip? It has almost arrived. CMOS is an acronym for complementary metal-oxide-semiconductor. It is a technology that now permits a designer to achieve (almost) the speeds of n-MOS but with one-tenth to one-hundredth the power dissipation. It appears that almost all of the new VLSI developments are in CMOS, CHMOS, and related technologies. By 1990, it is predicted that application-specific ICs will command 25% to 30% of the total IC market.

The May 20, 1985 issue of **Electronics Week** reports on the Custom Integrated Circuit Conference in Portland, Oregon. Shown in Figure 2 is the Toshiba "microengine," a CMOS version of the Z-80 microprocessor that includes interface circuits, clock generator, and a 3500-transistor custom macrocell. "It took only four weeks to complete the design through the mask data-base generation phase, and the first sample met all specifications."

In the June 24 issue of **Electronics** (pp. 58-63), "IC-Design Automation Strides Into Silicon-Compilation Era" describes how more conventional chip-design tools get boost from hardware accelerators and expert-system technology. "Entire LSI functions have been captured in huge standard cells VLSI Technology Inc. calls Megacells. To avoid wasting silicon real estate, all the firm's Megacells conform to a standard height and tie to the on-chip Megabus, which runs above and below them." You can detect our hardware bias in these items on system-on-silicon design. IC technology is the engine that drives most of the fastest growing segments of the computer industry. Megacell technology presages the ability to provide equal or higher performance computer and embedded-computer systems at ever lower cost in ever smaller packages. A firm such as DEC remains isolated with its LSI-11 and VAX product lines, which are not based upon standard, commodity microprocessors and programmable functions.

Speaking about DEC, **Electronics Week** (May 27, pp. 68-70) describes DEC's latest product, the MicroVAX II or VAXstation II. The $19,000 system challenges the

VAX-11/780 in CPU performance, and uses the VAX-on-a-chip processor, formerly called the MicroVAX 78032. "The 32-bit chip contains 125,000 transistors, but it is an n-MOS and not a CMOS device. The decision to use n-MOS was made at the start of the 33-month development process in 1982. At that time, explained Bob Supnik, MicroVAX II-chip project manager, DEC was reluctant to risk development work in CMOS technology. 'Future technology will be CMOS,' he says." Within the next several years, DEC will have to learn how to sell MicroVAX systems below $7000 if it wishes to remain competitive with 32-bit systems based upon chips such as the 80386 and 68020 as well as systems based upon megacells, macrocells, and the like. The improvement in price/performance ratios of low-end computer systems is proceeding much faster than DEC would desire.

IEEE Communications Magazine regularly publishes features of interest to a broader group of readers. In the July 1985, "Security in High-Level Protocols, by V. L. Voydock and S. T. Kent, provides a succinct discussion of basic concepts of data encryption. Jargon that is explained includes cipher, encipherment, encryption, encryption algorithm, cleartext, plaintext, ciphertext, invertible, conventional ciphers, public-key cipher, block ciphers, stream ciphers, and electronic code book (ECB). In the August 1985 issue, F. N. Parr and P. E. Green, Jr. discuss "Communications for Personal Computers."

D. M. Vaidya describes a "Universal RS232C Cable," in Microprocessors and Microsystems, June 1985. Something along this line is also available commercially. It is considerably easier, from both a hardware and software standpoint, to hook up a peripheral with a Centronics-type I/O port than with a RS232C serial port.

Mini-Micro Systems (July 1985) reviews desktop multi-pen plotters such as the Houston Instruments PC Plotter 695, the Hewlett-Packard 7470A and 7475A, and the IBM XY/749 Digital Plotter. Also mentioned is the Hewlett-Packard 7510 Color film recorder, which uses vector technology instead of raster technology. Instead of drawing on paper with ink, the HP 7510 draws on film with light. There are 15,344 by 10,895 addressable points per frame with over 16 million available colors. Cost? A paltry $13,900. You need lots of memory to take advantage of the HP 7510. We have used the Hewlett-Packard 7470A; it is superb.

Phil Wiswell, in "Word Processing: The Latest Word" (**PC**, August 20, 1985), puts eighteen popular word processors through a series of rigorous benchmarks. Included in this survey are: WordStar Professional, WordStar 2000, XyWrite II-Plus, Word Perfect, Volkswriter Deluxe, DisplayWrite 2, DisplayWrite 3, EasyWriter II System, SuperWriter, Perfect Writer, Microsoft Word, MultiMate, Samna Word III, OfficeWriter, Textra, Spellbinder, Personal QWERTY, and PFS:Write. The author recently obtained a copy of SuperWriter for use with his IBM PC in his lab. The problem: new commands and menus to learn. Phil Wiswell correctly identified the problem associated with deciphering C D F G I M N R S X Z CR /TAB ESC , which appears in a small window across the bottom of the Superwriter screen. Perhaps many of you have more stamina than the author, who is getting fatigued by the necessity to learn ever new commands for an increasing collection of "user friendly" software packages. Software command knowledge is steadily pushing out residual chemical engineering knowledge. We need a name for this phenomenon.

Five megamemory multifunction boards for the IBM PC AT are briefly described in the August 20, 1985 issue of **PC** (pp. 146-155). You can add combinations of 64K or 256K DRAMS to boards such as the Advantage! (AST Research, Inc.), SMF/AT210 (Sigma Information Systems), Grande Byte (STB Systems, Inc.), Rio Grande (STB Systems, Inc.), and Maestro (Tecmar Incorporated). 256K DRAMS are surprisingly cheap, in quantity, these days. **Business Computer Systems** (May 1985) provides an extensive listing of multifunction boards for the IBM PC. In the same issue of Business Computer Systems is a listing of new technology printers, the ink jet, thermal transfer, and laser printers (pp. 119). We prefer a nice laser printer, if we could afford it.

In **Byte** (May 1985), J. Markoff, P. Robinson, and D. Osgood discuss "homebrew chips," VLSI chips that you design yourself. A Syracuse University "AI coprocessor chip was actually fabricated through MOSIS (MOS Implementation System), a brokerage that connects chip and board designers with chip and board fabricators. MOSIS is an outgrowth of both the Arpanet and an idea from Xerox's Palo Alto Research Center. . . MOSIS will make two or more if you send them your design in either CIF (Caltech Intermediate Format) or Calma-GDS 2-stream format." There are about 900 chips per run; all you have to pay is your proportional share, which may be $5000 for a batch of 20 chips.

Bruce D'Ambrosio discusses "Building Expert Systems with M.1" in the June 1985 issue of **Byte** (pp. 371-375). M.1 is a knowledge-engineering tool for the IBM PC that costs a modest $12,500. Of course, if you wish a scaled-down version of the program, you need plunk down only $2000. **Electronics** (June 24, pp. 50-51) briefly discusses Gold Hill Computers and their software, Golden Common Lisp, which runs on an IBM PC. No price is given. Your author is waiting for Borland Turbo Expert, which should become available for $69.95 in several years if Borland International remains solvent. By the late 1980s, expert system software should become as plentiful as word processing software is today.

Marshall D. Abrams provides a nice overview and technical discussion, "Observations on Operating a Local Area Network," in **Computer** (May 1985). Concepts discussed include DTE, DCE, interconnection, interoperability, broadband, virtual circuits, datagrams, internets, bridge, name service, file transfer, flow control, speed conversion, error control, echoing, data forwarding, code conversion, protocol conversion, resource sharing, and so forth.

Our chemical engineering colleagues—Mordechai Shacham, Michael B. Cutlip, and Paul D. Babcock—have teamed up to contribute an article, "Simulation Package for Small-Scale Systems," in **Microprocessors and Microsystems** (March 1985, pp. 76-83). CAST Communications has been given permission from the publisher and authors to reprint this article in the spring 1986 issue. You may be interested in "C—An Alternative to Assembly Programming," which appears in the April 1985 issue of the same magazine (pp. 124-132).

Mini-Micro Systems is a good source for product listings in well-defined categories. The Spring Peripherals Digest issue (April 19) surveys disk drives, printers, tape drives, and graphics terminals; the Computer Digest issue (June 14) surveys single-board, single-user, multi-user and mini-computers; and the Communications Digest issue (February 15) surveys modems, multiplexers, local area networks, networking software, and voice/data computer/terminals. Micro-to-mainframe links are discussed in two articles in the May 1985 issue; a NOVA-compatible reduced instruction set computer (RISC) system is briefly described in the same issue. More on RISCs later in this column.

In the May 1985 issue of **PC Tech Journal**, "Reflections of Unix" discusses PC/IX, VENIX/86, XENIX, COHERENT, QNX 1.2, and uNETix SFS 2.0. Tables 2-4 compare the availability of 193 different UNIX System III commands, including system administration, text processing, and programming development commands in the six software packages. One-hundred ninety-three commands? Ugh! Unix is an operating system that seemingly only a computer scientist could love.

PART 3

"Word Processing Programs: Bundles of Functions," in **Business Computer Systems** (March 1985), compares the features of 57 different word processors. This listing gives us an opportunity to add a sixteenth "irrefutable law" of computer systems: 16. A comparative listing of 50 different software packages will not contain the software package that is of interest to you. PeachText 5000, the one we use, is not mentioned. Actually, the value of software becomes apparent when it is tested. At Virginia Tech, a room in our conference center is dedicated to the testing of personal computer hardware and software. About 15 different types of PCs as well as 40 to 50 different, major software packages are represented (all donated). The author is becoming tired of writing about articles on word processing software; perhaps a moratorium is in order for this column . . . for five or ten years.

Byte has done it again with its excellent special issue on Artificial Intelligence (April 1985). Articles include "Communication with Alien Intelligence," "The Quest to Understand Thinking," "The LISP Tutor," "Proust," "Architectures for AI," "The LISP Revolution," "The Challenge of Open Systems," "Vision," "Learning in Parallel Networks," "Connections," "Reverse Engineering the Brain," "The Technology of Expert Systems," and "Inside an Expert System." Also discussed in the same issue is "A Million-Point Point Graphics Tablet," or how to convert the KoalaPad for use with the Zenith Z-100 PC.

"What's Wrong with Computer Graphics: Tufte Talks Chartjunk and WYSIWYG" is the feature article in the April 1, 1985 issue of **Datamation**. Says Tufte, a noted statistician and information designer: "Too much chartjunk. No sense of visual craft. What good are 4028 colors without [the user having] any sense of color? What good are 22 type fonts if they all have jaggies? Computer graphics has tremendous potential, but for several reasons it's largely unexploited." Tufte believes that in many cases the application of a computer to graphics has been a step backward, "for in the change from monotype to microcode much of the graphical wisdom accumulated since Gutenberg began printing books 500 years ago has been lost." The author immediately purchased Tufte's book, **The Visual Display of Quantitative Information** ($34 postpaid. Send check or money order. Available only by ordering directly from Graphics Press, Box 430, Cheshire, CT 06410) and was well rewarded. One of the important messages of the book is that most figures are too cluttered and hide, rather than emphasize, the important message that the graphed data provides. Tufte's ideas should be required reading for all chemical engineering students. The book makes an excellent gift; a couple of months ago the author saw of stack of them in the office of his CACHE colleague, John Hale (DuPont, Wilmington).

Dr. Dobb's Journal, March 1985, is a Special Prolog Issue. Three articles are provided: "Programming in Logic," "Tour of Prolog," and "Tax Advisor: A Prolog Program Analyzing Tax Issues." A fifteen-page listing is associated with the Tax Advisor article, which was the winner of Dr. Dobb's AI programming contest and "is a program that knows how it knows what it knows, and why it wants to know what it doesn't know." This is the type of issue that makes Dr. Dobb's such a fine magazine. G. A. Edgar discusses "A Compiler Written in Prolog" in the May 1985 issue of Dr. Dobb's. A complete listing is given for the 8080 microprocessor instruction set in Micro-PROLOG, which is available on a CP/M Z80, MSDOS, PCDOS, CP/M-86, and Unix.

The February 1985 issue of **IEEE Control Systems Magazine** is a special issue on Future Directions in Control Systems. You may be interested in the article, "Control Engineers Workbench—A Methodology for Microcomputer Implementation of Controls."

Fault Tolerance is the subject of an article, "Computers That are 'Never' Down," in **IEEE Spectrum** (April 1985). For you 'smart-home' buffs, the May 1985 special issue of **Spectrum**, "At Home with High Technology," may be of interest. Would you believe a house that ."will contain 10 IBM computers on a local area network, an Apple IIe, and two Apple Macintoshes?" The logical defense to this seemingly absurd circumstance is, "You can never have too many computers." Read about it in "Portia's Perfect Pad: Superhigh Tech," on page 56-63. This is the type of magazine that CEP should strive to become.

No column is complete without mentioning our favorite computer industry gossip, sage, and seer, Felgercarb N. Eloi, the editor of **DTACK GROUNDED** (The Journal of Simple 68000/32081) who is known, with or without affection, to subscribers as FNE. In Issue Nos. 42 through 44, covering the period June through August 1985, FNE discusses topics such as "Mackintosh meets IBM PC Guru Norton," "Jacki (Jackintosh) and GEM," "ATT's 32-bit micro chip set," "The Very Strange World of DRAM Pricing," "C HLL OVERHEAD (by Otherwise Intelligent)," "More DRAM Pricing Wars," "The p-System: REQUIESCAT IN PACE," "Tandon Lawsuit and Apple 800K floppies (?)," "32-Bit Micros," "4-layer printed circuit boards," "Mackish Color Graphics Revisited," "Monochrome Graphic CRT Monitors," "Color Graphic CRT Monitors," "Nat'l Semi's 32000 series: third party views," "Wild, repetitive, incoherent ravings," "RISC architecture—our first look," "CHEAP MEMORY—HONEST!," "RULE BRITANNIA (Inmos woes), and others. See the next item for RISC comments. [Subscriptions are $15 for 10 issues in the U.S. and Canada (U.S. funds) or $25 for 10 issues elsewhere. Make check payable to DTACK GROUNDED, 1415 E. McFadden, Ste. F, Santa Ana, CA 92705.]

The August 1985 issue of **IEEE Spectrum** features an article, "Toward Simpler, Faster Computers," that probes the advantages of reduced-instruction-set computers (RISCs). The object is to minimize the number of different instructions but provide numerous internal registers so that data need not be swapped between the CPU and memory so often. Those who question the approach make the following points: (a) "RISCs require larger programs than complex-instruction-set computers (CISCs) to do equivalent problems, (b) RISC instruction sets have been pared down to the point where certain operations that might take only a few instructions on a conventional computer require complex subroutines, and (c) RISC principles make no use of the increasing density available with advances in integrated-circuit technology." Felgercarb N. Eloi remains to be convinced that a RISC makes sense. Comparing a CISC to a RISC is like comparing apples and oranges. A RISC is faster than a CISC, but the former needs its increase in speed to handle the additional memory fetch operations. As FNE states, "WE STRONGLY SUGGEST THAT YOU IGNORE THE MIPS RATING OF RISC MACHINES! RISC machines HAVE to have a high MIPS rating just to get out of their own way!"

GUIDELINES FOR USING THE IBM-PC IN THE LAB

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Liscouski [1] has outlined two general uses of computers in the laboratory: instrument or experiment automation and laboratory management systems. In both industry and academia, the IBM-PC series of personal computers has become ubiquitous for the latter function, but has not been as commonly used for the direct automation of instruments, including the collection of experimental data. We therefore will address this article to the question of how the IBM-PC can be best utilized in a laboratory setting for data acquisition and instrument control, and then briefly discuss the advent of integrated systems that combine both automation and laboratory management functions in a single package. The details of adapting an IBM-PC for use in the laboratory can be usefully divided into two sections: hardware and software.

HARDWARE

There are numerous manufacturers of data collection boards for the IBM-PC. How does one decide which manufacturer's hardware to purchase, or indeed which of the several boards from a given manufacturer are appropriate? Most often, data collection and control is done using either a board containing an analog- to-digital converter (A/D), digital-to-analog converter (D/A), timers and digital input/output capability, or, where these functions are built into the instrument to be interfaced, a board implementing the IEEE-488 (GPIB) functions. The IEEE-488 standard was developed for Hewlett-Packard instruments, but an increasing number of other manufacturers is choosing to use IEEE-488. The IEEE-488 interface is well standardized and should be used when available on the instrument you are interfacing. A less powerful, but still useful choice is the RS 232C (serial) interface, which is used by some instrument manufacturers. If neither of these choices is available on the instrument, then the designer must develop an interface using A/D's, D/A's, digital I/O, timers and other devices; unfortunately there is no standard for these, and the array of choices can be almost bewildering.

If you are going to use an A/D for data collection on the IBM-PC, it would appear that a primary consideration is the speed at which data can be collected. Although the situation seems to change almost daily, it is our experience that the IBM-PC, excluding the AT version, is suitable for routine data collection at rates up to approximately 40 kHz. With special programming and hardware, rates of up to 95 kHz are possible. An assembly language routine capable of inputting data at slow to moderate rates has been previously published [2]; a short routine to achieve maximum rates above this is shown in Listing 1. Rates much above 95 kHz appear to be difficult to achieve because of the inherent speed limitations of the 8088 processor used in the IBM-PC (at 4.77 MHz clock speeds) and its 8-bit data bus. When appropriate hardware becomes available, therefore, the IBM-PC/AT, with its 80286 processor and 16-bit data bus, should be capable of much higher data rates.

Two features associated with the A/D require particular attention. One is the resolution of the A/D. Most A/D's currently used for scientific data collection are probably 12-bit A/D's. Although commercially available, eight-bit A/D's provide inadequate resolution for any but the least exacting work. Some instruments which report data over an extremely wide range, or for which small changes in output are important, may well necessitate the 14-bit or 16-bit A/D's available from some manufacturers. The major tradeoff here is resolution versus speed and cost; 16-bit A/D's are typically more expensive and operate less rapidly than 12-bit A/D's.

The other major feature that differentiates several manufacturers' A/D's is the manner in which data collection is accomplished. Three methods are commonly used on the IBM-PC: direct program control, interrupt-driven data collection, and direct-memory-access (DMA). The simplest to use is the first method, in which the program initiates the data collection (or a timer may do so), and then waits until the datum is available, stores it, and then waits until time to initiate the next data collection cycle. Under interrupt-driven data collection, once the data collection process is initiated, the main processor of the Im tasks other than just data collection; these other tasks are interrupted whenever a timer signals that it is time to collect another datum. DMA is similar to interrupt-driven data collection, except that the data are stored in memory by a processor on the A/D board, rather than by the processor in the IBM-PC; hence, this technique places the lowest demand on the central processor.

With the boards currently available for the IBM-PC, it would appear that for rates of up to approximately 1 kHz, any of the three methods can be used. However, although it is certainly the simplest method for the programmer to handle, direct program control is the least preferable because it permits only one program or task to be executed, namely data collection, whereas the other methods permit one or more other processes to occur asynchronously to data collection. At rates of 1 to 5 or 10 kHz, interrupt-driven collection becomes less and less efficient, as proportionally more time is spent on the overhead of handling the interrupts.

At rates of approximately 10kHz and above, interrupt-driven data collection is not possible. Boards are not yet widely available that use DMA at rates much above 25 kHz, although there is no apparent reason why this has to be true, since rates of up to 238 kHz should be possible with the DMA circuitry in the IBM-PC (3). Hence, at rates of 25 to 95 kHz, direct program control method is the usual choice. Incidentally, it should be noted that the rates described here refer to aggregate rates, i.e., the rates of all "channels" of data combined, and these limitations will not necessarily hold for the IBM-PC/AT or other higher-speed computers, or to new A/D's undoubtedly currently under development.

Other features that the user may wish to examine about a particular A/D include immunity of the board to noise, the physical ruggedness of the board (especially in industrial environments), and the availability of programmable gain. In addition, for some applications, the user may wish to consider integrating A/D's (for relatively slowly-changing signals in a electrically noisy environment), or flash or other high-speed A/D's where extremely high speed (but usually reduced resolution) may be required.

For a general-purpose scientific or industrial system, a good choice of A/D is a 12-bit A/D with programmable gain (between 1 and 1000), maximum speed in the 10 to 40 kHz region, and multiple inputs that can be configured in the differential input channel mode. This will permit data collection from an extremely wide range of instruments; a board with these specifications is available from most major manufacturers of boards used for scientific and industrial applications.

The other features of these boards do not vary nearly as much as the A/D. Usually, there is a 12-bit or higher resolution D/A to allow for the driving of oscilloscopes, recorders and other analog devices. In addition, a useful addition is 8 to 16 bits or more of digital input/output capability; the usual function of these is to sense switch closures and to activate other devices via relays. Finally, the boards usually contain one or more timers (or clocks), which can be used to time both the input and output functions of the board; for example, a timer is usually used to regulate the speed of data collection. Such timers should be able to achieve very high rates (in the MHz range) to assure precise timing of events. A useful feature is also some sort of line-frequency clock. Collection of data at some multiple of the line frequency will often help reduce much of the "noise" picked up on analog lines in the system; this applies only to signals collected at frequencies less than the line frequency.

Another item of hardware necessary for scientific applications is the floating point coprocessor (the Intel 8087 series). Because data collection typically involves only 16-bit integers, a floating-point chip is not required for data collection alone. However, the 8087 significantly speeds the calculations that are usually performed on such data (e.g., fast Fourier transforms); depending upon the language and the application, I have observed 30% to 400% improvements in the speed of execution of scientific application programs. Hence, it is useful to add the 8087 to almost any system where scientific applications are routinely used. It should be pointed out, however, that not all scientific software on the IBM-PC utilizes the 8087.

Depending upon the application, the user may also wish to purchase one of the special-purpose boards for the IBM-PC, including such things as digitizer, optical isolation board, ultra-high speed data collection boards, boards for processing video or audio data, stepper motor controllers, or similar devices. In any case there appears to be as wide a range of hardware accessories available for the IBM-PC as for most other computers used in the laboratory. Thus, other than the upper limit on speed, the hardware available for the IBM-PC seems to make it suitable for almost any application.

SOFTWARE

One of the measures of the success of a laboratory computer is the availability of a wide variety of software. Although the IBM-PC has been on the market a relatively short time, the amount of scientific software continues to grow quite rapidly. Most of the companies which market data collection boards for the IBM-PC have available software to utilize their own hardware, and certainly the user will wish to purchase such a package of software unless he or she has very special needs; writing data collection software, usually in assembly language, is not an easy task even for an experienced programmer.

Certainly, wherever possible, the scientist should avoid writing software that duplicates commercially-available software; the labor cost of writing it yourself is inevitably far greater than the cost of even "outrageously-priced" software. "Free" software from colleagues may also involve hidden costs in the form of time needed to adapt it or correct programming errors.

Having said all of that, however, we must still admit that we, like many scientists, prefer to write our own software, because of the freedom it gives us to customize it to our own needs. Our preference for the IBM-PC hand has excellent graphics support. However, the recent introduction of graphics support for other languages by IBM, and the continued introduction of more efficient compilers and more extensive "tool-kits" providing commonly-utilized routines makes the use of other languages increasingly attractive. Data collection routines are still usually written in assembly language, but these can be linked to programs in higher level languages that perform all of the remaining data storage and processing functions.

As two examples of the ease with which programs for use in laboratory data collection and analysis can be developed with IBM's BASICA language, we would like to describe two programs which were initially developed by students as part of a 3-week computer interfacing course, and which are now used in our analytical chemistry laboratory class on a routine basis.

The first of these is a program to collect and integrate data from an isocratic HPLC system. Because the output from the UV detector in our system (a Beckman 330 filter UV detector) must be amplified by a factor of 1000, noise levels in the amplified signal are fairly high and require some filtering, both in hardware and software. Other than this requirement, the data collection is very straightforward and uses a standardized data collection routine [2]. Data collection is usually at 2 Hz, so that the HPLC peaks normally contain 50 to 100 data points each. Data are stored in permanent disk files, and contain the HPLC and data collection conditions as part of the files. These conditions are also stored in a separate file, so that the operator does not need to reenter them for each sample. Integration is done with standard software techniques, and allows for use of internal standards and labeling of known peak identities. An example of the output is shown in Figure 1.

A second example of a student-written program is one for analysis of polarographic data. Again,the data collection portion of the program is quite routine; the challenge to the programmer is in putting the data into chemically useful form. This particular program will analyze data from either DC polarography or differential pulse polarography; the students in the analytical lab run the same sample in both modes and compare the results. An example of the output from this program is shown in Figure 2. The most challenging portion of the program for the student to write was the portion fitting lines through the three major portions of the curve, even though the data are in a "saw-tooth" form.

FUTURE TRENDS

There are two major trends which appear to be in the near future for laboratory computing using the IBM-PC; both are trends which take advantage of the higher speed, larger memory and large user base of the IBM-PC compared to other microcomputer systems. The two emerging trends are toward foreground/background systems and integrated data management.

In the foreground/background systems, laboratory data collection is carried out simultaneously with data analysis or other functions. This is accomplished using either the interrupt-driven data collection or DMA data collection processes mentioned earlier. The IBM-PC implements an 8-level prioritized interrupt system (using an Intel 8259 interrupt controller), so that interrupts from several sources may be conveniently handled. It also has a four-channel DMA controller (implemented with an Intel 8237-5 DMA controller). Hence, either or both of these approaches may be used to allow simultaneous data collection and data processing. A typical application is the collection of data from one experiment while the data from a previous experiment is being processed. Such foreground/background systems are available from many manufacturers of data collection systems. However, in most such systems, the non-data collection process must also be a program written by the user; that is, true multitasking has not been widely implemented on the IBM-PC for data collection. Multitasking systems, such as Unix-based systems, are available, but probably will not be widely used in laboratory applications, because of the complexity and high overhead (in execution time) of such systems.

The second major trend is toward systems that integrate data collection with data processing. There are now several software packages available which integrate laboratory data collection with data display and data manipulation routines; for example, the data may be smoothed, integrated, differentiated, and transformed by Fourier or other techniques. Such packages may also allow plotting of data on hard-copy plotters, and may have provisions for storage of laboratory notebook information pertinent to each sample analyzed. Simple statistical techniques may also be applied to the data.

These packages may also allow use of data base management and other techniques more familiar to those in business settings. Essentially, these systems implement commercially what has been done in major industrial laboratories for many years, namely, a method for storing, processing, and retrieving data for use in proprietary data bases, except that no large central computer system is necessarily involved. Presumably, with the movement toward networking that is being encouraged by the large computer manufacturers, including IBM, many versions of these integrated software packages will include the ability to move data to the large mainframe computers for archiving or further processing. However, in contrast to earlier systems, the microcomputer will be the major locus of data processing, rather than just the collector of the data and a smart terminal to a more sophisticated system.

SUMMARY

Overall, then, the IBM-PC can be easily adapted for use in the laboratory. The extensive base of commercial software and hardware for this system makes it useful in an extremely wide range of applications. Particularly with the advent of foreground/background systems and integrated data collection and data management systems, it would appear that the IBM-PC is a useful addition to the list of computers that can be used in the laboratory. And we look forward to the development of hard-disk-based 16 or 32-bit systems with higher clock speeds, and of low-cost dedicated array processors, to make the IBM-PC series even more widely useful in the laboratory.

Literature Cited

[1] J. G. Liscouski, "Planning an Approach to Laboratory Automation," in J.G. Liscouski, ed., **Computers in the Laboratory**, American Chemical Society, Washington, D.C., p. 1, 1984.

[2] S.C. Gates, "Laboratory Data Collection with an IBM PC," **BYTE**, May, 1984, pp. 366-378.

[3] L.C. Eggebrecht, **Interfacing to the IBM Personal Computer**, Howard W. Sams & Co., Indianapolis, p. 188, 1983.

Figure 1

Isocratic high performance liquid chromatographic analysis of caffeine in a commercial cola drink by a student in the senior-level analytical chemistry class. Peak 1 is the caffeine, Peak 2 is benzyl alcohol, the internal standard. Areas shaded indicate the areas integrated by the HPLC computer program. Peak 1 was reported to be 1.13 times the area of peak 2.

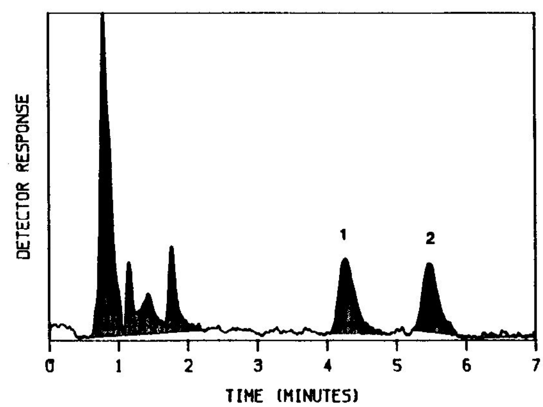
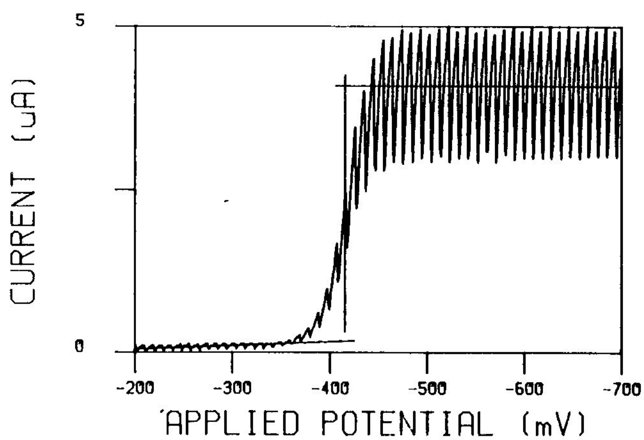


Figure 2

DC polarographic analysis of a 0.5 mM lead standard solution by a student in the analytical chemistry class. The straight lines through the data indicate the computer fits to the two sections of data, with the vertical line passing through the computed inflection point. The distance between the two horizontal lines along the vertical line is proportional to the concentration of the sample; in this case, the difference is 4.05 uA, and the half-wave potential (inflection point) is at -415 mV, according to the report produced by the program.



CACHE REPRESENTATIVES RECEPTION CHICAGO AICHE MEETING

The annual reception and program for CACHE representatives and their guests will be held from 5 to 7 p.m. on Wednesday, November 13, 1985, in the Upper Exhibition Hall, 4th floor, in the Palmer House Hotel at the Chicago AICHE meeting.

CACHE President, Professor Richard S. Mah, will introduce Task Force chairmen and briefly review the CACHE activities and accomplishments. Two of the on-going CACHE projects will be highlighted. Professors Morton Denn and Warren Seider will discuss CACHE initiatives undertaken by the Curriculum Task Force. Professors Manfred Morari and Ignacio Grossmann will briefly describe the new Process Design Case Studies and their relationship to computer-aided design techniques.

Other attractions will include display and demonstration of software for personal computers and mainframes for chemical engineering education, electronic mail, poster stations on artificial intelligence and expert systems, and optimization capability in FLOWTRAN. Also on display will be several recent CACHE publications: conference proceedings, design case studies, position paper for Computing in Chemical Engineering Curriculum.

Details on the reception will be sent to all CACHE representatives and Chemical Engineering Department chairmen prior to the meeting. Individuals and companies who wish to participate in the poster session should contact:

Professor Ignacio E. Grossmann
Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
(412) 578-2228

After the reception, CACHE Trustees will arrange for informal dinner groups for all attendees who wish to discuss their particular interests.

LARGE SCALE SYSTEMS

Jeff Siirola
Eastman Kodak Company

The Large Scale Systems Task Force is continuing to make progress on two projects which should be of some interest to educators involved in process design and simulation. The first of these is the development of an optimization capability enhancement of the CACHE FLOWTRAN simulation program. This project is being directed by Professor Lorenz Biegler of Carnegie-Mellon University. Dr. Dan Schneider of Monsanto Company has also generously provided technical assistance.

The optimization scheme is to employ the "infeasible path method" previously developed by Professor Biegler. A prototype system has been programmed and tested on several simulations with excellent results. A more convenient interface with the CACHE FLOWTRAN program is now under development at CMU and Monsanto. The resulting system will undergo further thorough checkout throughout the Fall. Upon completion of this testing phase, Professor J. D. Seader of the University of Utah will assist with the development of the most efficient means of distributing the optimization enhancement to CACHE FLOWTRAN users. The documentation for the enhancement will be included in the next edition of the FLOWTRAN manual to be published in 1986.

The second LSSTF project involves yet another effort to bring additional design and simulation tools to the educational community. Professor G. V. Reklaitis of Purdue University is attempting to secure for CACHE the program SPEEDUP, an equation-based steady state and dynamic process simulation program developed at Imperial College by Roger Sargent, John Perkins, and their coworkers. Negotiations are currently underway with the British Technology Group, which holds the rights to the program, to enable CACHE documentation and distribution of SPEEDUP load modules to interested institutions in a manner similar to the distribution of CACHE FLOWTRAN. Further progress on this project will be reported next issue.

TASK FORCE FOR THE DEVELOPMENT OF PROCESS DESIGN CASE STUDIES

Manfred Morari—Caltech
and
Ignacio E. Grossmann-Carnegie Mellon University

The CACHE Task Force on Process Design Case Studies under the direction of Professors Manfred Morari and Ignacio Grossmann has completed several activities. The case study "Separation System for Recovery of Ethylene and Light Products from a NAPTHA Pyrolysis Gas System" has been completed by Ignacio Grossmann and can be obtained for $15 by writing to

Professor Brice Carnahan
Department of Chemical Engineering
University of Michigan
Ann Arbor, MI 48109

The report includes preliminary design calculation by hand, detailed computer simulations, and it illustrates the application of process synthesis techniques for separation and heat exchanger networks. The problem of this case study was supplied by Dr. Dan Maisel from Exxon Chemicals.

Two other case studies have been completed and are being printed currently. They are scheduled to be available for purchase around the middle of November.

Case Study 2: "Design of an Ammonia Synthesis Plant"

The objective of the case study is the design of an ammonia synthesis plant that is to be built in 1990, and that uses hydrogen and nitrogen feedstocks from a coal gasification plant. All stages of the design procedure starting from preliminary calculations down to the detailed flowsheet calculations are described. The proposed design incorporates a medium pressure synthesis loop with water adsorption/distillation for ammonia recovery and with membrane separation for hydrogen recovery. The process was designed with the simulator PROCESS from Simulation Sciences and the ammonia reactor was designed with a special purpose package QBED. A listing of this program is included in the case study. Depending on the required detail and the availability of process simulation software, the case study is suitable as a one term assignment for a single student or a group of students.

The problem statement was supplied by Philip A. Ruziska from Exxon Chemicals and the case study was prepared under the supervision of Ignacio Grossmann.

Case Study 3: "Preliminary Design of an Ethanol Dehydrogenation Plant"

The objective of this case study is a preliminary design of an acid aldehyde synthesis process by ethanol dehydrogenation. The project covered all stages of the design procedure starting from consideration of qualitative aspects of the flowsheet and preliminary calculations to detailed process simulations and final economic evaluations. In this study, emphasis is placed on synthesizing a workable flowsheet and justifying its configuration, simulating and evaluating the design using commercial process simulator and deriving a heat recovery network for the final process.

The study revolves around the simulation of the flowsheet using PROCESS from Simulation Sciences. Some of the features, advantages and limitations of this simulator are presented. The study concludes with a complementary presentation of this process simulated with the CACHE version of FLOWTRAN. While the aim of this study is not to provide a detailed comparison between PROCESS and FLOWTRAN a useful description of the relative merits of both simulators can be readily observed.

The project is suitable for a one term project by a 5 or 6 person team of senior design students. The results of two such teams are given in this study. This problem was posed by Union Carbide Corporation and the case study was prepared under the supervision of Professors L. T. Biegler of Carnegie Mellon University and R. R. Hughes of the University of Wisconsin.

Statements for the new case studies will be available by December, 1985. For information on these design problems or for anybody interested submitting a report for publication, please contact:

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California Institute of Technology
Pasadena, CA 91125
(818) 356-4186

or

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Department of Chemical Engineering
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ZPLOT—GENERAL PURPOSE GRAPHICS PROGRAM FOR THE IBM PC

ZPLOT is a stand alone interactive program to generate XY plots from data files. The pıogram is unique in that 95% of the parameters specifying the plot can be accessed and changed by the user at run time. This results in great flexibility which can be utilized after minor experience with the program. For all plot parameter choices, reasonable default values are provided.

ZPLOT divides the physical screen in "windows" on which diagrams are placed. Each diagram consists of axes, labels and curves. Several diagrams can be placed on top of each other, thus allowing special effects like multiple Y scales with Y axes shown both on the left and right side of the diagram. It is possible to switch between linear and logarithmic axis scales at the touch of a key. Major and minor grids can be drawn, labels can be placed anywhere on the diagram or automatically centered along the axes.

Hardware:

IBM PC or compatible running under DOS 2.0 or later operating system. Most major monochrome and color graphics boards are supported, e.g., IBM, Hercules and AMDEK.

Hard copy devices:

Any dot matrix printer can be used if a user supplied run time interrupt routine is available. Furthermore, multicolor pen plotters manufactured by Bausch and Lomb and Hewlett Packard are supported.

The program can be obtained for a single user price of $75 from Manfred Morari, Caltech, 206-41, Pasadena, CA 91125. Please include a check with your order. Purchase orders cannot be accepted. Site licenses are available, please inquire.

SURVEY OF MICRO- AND PERSONAL COMPUTER APPLICATIONS IN THE LABORATORY

Easy-to-use micro- and personal computers have been available for several years now and many chemical engineering faculty have discovered that off-the-shelf interfacing equipment often can be used to build a relatively inexpensive on-line system for acquisition and analysis of process data. Such systems are widely used in research laboratories; recently they have been introduced into undergraduate laboratories.

A properly-designed system, i.e., computer and experimental unit, can greatly enhance the quality of the undergraduate laboratory experience: the student can interact effectively with the on-line system to operate (control) the experiment as desired. More data can be obtained, tested for consistency, and creatively analyzed than by using traditional methods. Effective use of graphics can also help in the student/experiment interaction; and professional quality graphs can be prepared by the machine to document student results.

A poorly-designed system, conversely, can be worse than a traditional "bad experiment". If the system introduces major errors in the acquired data, does not operate consistently, or does not materially aid in analysis of results, the student may invest a lot of time and obtain relatively little understanding of the experiment. Even if the hardware works efficiently, the software may be "user-unfriendly" or may furnish the student with the ultimate cookbook laboratory experience....."(1) push key to start, (2) collect analyzed results."

Good laboratory experiments that incorporate an on-line computer require a lot of creativity in designing them; and they require hard work in building, testing, debugging, and documenting them. We all agree that successful efforts in this area deserve much broader dissemination than they routinely receive. As a profession, we need to modernize and make greater use of our undergraduate laboratories; even large departments can use some assistance in this area. Perhaps as important, the individual faculty members who take the time to develop such facilities deserve professional recognition. Junior faculty, who often have the required skills and experience to make such contributions, are dissuaded from investing the effort because of the lack of recognition and rewards that accompany successful work in this area.

CACHE would like to assist the development of this important area. As a first step, the Micro Software and Systems Committee proposes to identify the significant developments that have already been made in individual departments. A simple survey has been designed by Professor Ali Cinar of the Illinois Institute of Technology that will be mailed out to department heads and CACHE representatives. If you have developed a facility or facilities in this area and want other faculty to know about them, please make sure your work gets reported on the questionnaire, or directly to us.

As a second step, based on compilation of the survey results, CACHE will undertake to publish concise descriptions of the most significant experimental developments. Publication may take the form of a series of brief articles in the Newsletter or as a separate published volume (monograph) dealing exclusively with the application of micro- and personal computers in the laboratory. The purpose will be to disseminate basic information on the most imaginative applications of on-line computers while recognizing those faculty who have contributed. Copies of the survey or further information may be obtained from:

Professor Ali Cinar
Dept. of Chemical Engineering
Illinois Institute of Technology
Chicago, IL 60616

or

Professor Duncan Mellichamp
Dept. of Chemical Nuclear Engineering
University of California
Santa Barbara, CA 93106

PHASE EQUILIBRIA PROGRAMS FOR APPLE II+

by Ricardo Reich
Universidad de Concepción, Chile

Two new phase equilibria programs are now available for the APPLE II+ microcomputer: ASOG and MINISIPRES.

ASOG calculates phase equilibria for the vapor-liquid, gas-liquid, solid-liquid, and liquid-liquid cases when evaluating the activity coefficients in the liquid phase by the ASOG method. In addition, it considers for some applications the UNIFAC method and the two-parameter Wilson model. The program structure considers a data bank (on diskette) with random access that enhances the calculation process and that contains 150 fluids basic properties, ASOG and UNIFAC structures (when available) and Antoine vapor pressure constants. The program includes the most recent ASOG and UNIFAC interaction parameter matrix. Program execution is interactive and user-friendly, with several options given in a menu. This program, in BASIC, is available with Spanish or English dialogs and requires only one disk drive.

MINISIPRES is a simplified version of a general thermodynamic property generator that is currently under development for larger computers. It is basically intended for energy balance calculations and second analysis. It therefore decides on the phase state of a process stream (liquid, vapor or both) by an isothermal flash and then calculates all its volumetric and thermodynamic properties (H, S, B, V and M). Two calculation methods are available to the options are again available for calculation. The Redlich-Kwong-Soave, Peng-Robinson and Lee-Kesler-Plocker equations of state are options for the first method; k_{ij}'s are automatic for the Lee-Kesler method but have to be entered by the user for the other equations. The Virial equation of state (truncated in B) is used for the vapor phase in the second method; B's are calculated by the Tarakad and Danner or Hayden and O'Connell methods. The Margules 3-s, van Laar, Wilson, NRTL and UNIQUAC models (with user-supplied interaction parameters) and the ASOG and UNIFAC group-contribution methods (with built-in structures and parameters) are used in the liquid phase. Interaction parameters are compatible with the DECHEMA VLE Data Collection. Other options included are the COSTALD method for the estimation of liquid densities, the generation of P-T-X-Y binary VLE tables, thermodynamic property tables, activity coefficient model parameters from infinite dilution and azeotropic data, and the administration of its data bank.

As in program ASOG, MINISIPRES considers a data bank for 150 fluids with many basic parameters that are required in the calculations. Minimum user-supplied data are required. Different systems of units are allowed (SI or English). Program execution is interactive and user-friendly, with input correction possibilities and standard output to a printer. This program, in BASIC, is available with Spanish or English dialogs and requires two disk drives.

Both programs are intended for teaching purposes in Chemical Engineering. Contact:

Professor Ricardo Reich
Dept. Chemical Engineering
Universidad de Concepción
Casilla 53-C
Concepción, Chile

COMPUTER PROGRAM FOR THE WATER STEAM TABLES

by Ventura Cerón and Ricardo Reich
Universidad de Concepción, Chile

A computer program for the generation of the VDI-Steam Tables (E. Schmidt, Springer Verlag, 1982) is available for teaching purposes in FORTRAN 77. The program execution is interactive and user-friendly and considers several options depending on the system of units required, phase state and independent variables given. Three systems of units are available: SI, metric and english. The program is divided in four zones: saturation, vapor, liquid and critical, and allows many combinations of independent variables: T(P, V, H, X); P(H, V, T); V(P, H); H(V, X); S(T, P, V, H, X). Thermodynamic properties given as output are T, P, V, H, U, S. In those cases, when iteraction is required, options by default or by initial value (user-supplied) are provided.

The program reproduces exactly the thermodynamic property values of the VDI (1982) and ASME Steam Tables (1967). The program, available on tape, can be supplied with Spanish or English dialogs.

Contact:

Prof. Ricardo Reich
Dept. Chemical Engineering
Universidad de Concepción
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Concepción, Chile

PC VERSION OF HYSIM SYSTEM

by T. Vysniauskas
Hyprotech Ltd.

HYPROTECH LTD. is a Calgary-based engineering software firm, which provides simulation software for a variety of oil companies and engineering firms. We are now pleased to offer the PC version of our process simulator, "HYSIM", to Chemical and Petroleum Engineering Departments at a special rate of $500 US per copy. If you were looking for CAE design programs then this offer may be of interest to you.

HYSIM is a generalized flow sheet simulator that is capable of simulating any unit or process configuration used in the oil and gas industry. The basic difference between HYSIM and other programs is that it is completely interactive. The user can progressively step through a simulation case by conversing with the program in common English commands, look at intermediate results, access a menu based help facility at any level in the program and modify or store the simulation case at any point. Data about specific streams can be entered at any time, in any order, and in complete free format. The property package within HYSIM will attempt to perform any calculations it can as stream information becomes available.

If you are interested in obtaining additional information, please write:

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EURECHA TEACHING PROGRAM PROJECT

The EURECHA Teaching Program Project is aimed at the collection and standardization of university chemical engineering computer programs, and the distribution of the modified programs to teaching institutions. The modifications make the programs suitable for almost all machines with FORTRAN compilers, and can be used interactively or in batch mode.

Short descriptions of the newest programs follow; descriptions of earlier programs are available on request. The earlier programs include CHEMCOSET: data bank; UNICORN: flowsheet program; DISTILSET: distillation programs; THERMDINSET: thermodynamics; CAPCOS: capital cost estimation package; TACS: simulation of control systems; and VLESET: comprehensive VLE analysis package.

Teaching institutions wishing to order any of these programs should write to the following address:

EURECHA
Technisch-Chemisches Labor
E.T.H. Zentrum
CH-8092 Zurich
SWITZERLAND

DIAGNOSE: Chemical Plant Fault Diagnosis Exercises

Authors: I.D. Doig, D. Himmelblau—a version of the CACHE Program

This package contains the simulated results from two different plants operating under correct conditions and also under a multitude of mal-functioning situations. The student is given his plant operating incorrectly, and he must perform tests to locate the error. Tests involve costs, and time also involves loss of profit, so there is adequate incentive for the student to think his trouble-shooting strategy through properly before requesting the tests by re-running the simulation. The multitude of mal-functions means that each student gets a different problem, and the more advanced exercises combine faults to provide even more alternatives.

One problem is concerned with a chlorination plant with two reactors, and the second plant is a distillation plant containing two columns.

The exercise has been used for many years at the University of New South Wales Australia, and has been distributed widely in the US by CACHE. It is particularly useful for courses that emphasise plant operation as opposed to the more traditional courses that emphasise plant design.

These process diagnostic execises are, in essence, an educational game, designed to encourage chemical engineering students to apply their acquired mass, energy and pressure balancing skills, and their knowledge concerning the distribution of the components of mixtures between liquid and gas (vapour) phases to resolve the cause (or causes) of a discerned mal-function (or distinct drift from normal desired behaviour) in a chemical plant. These exercises thereby serve a similar function to that served the process design problem in a typical chemical engineering course: they cause the student to bring many of the skills he has separately acquired in other parts of his course to focus in tackling a common chemical engineering problem. The exercises also teach a strategy for problems of the trouble-shooting kind.

SYNSET: Heat Exchanger Network and Column Sequencing Programs

Authors: Fonyo Z. and Rev E.
Technical University of Budapest

The SYNSET programs were developed to aid the teaching of process synthesis, the inventive step in the design where the chemical engineer selects the component parts and their interconnections to create a structure which can meet stated design requirements.

The set consists of two programs, the program HENSYN, and COLSYN.

PROGRAM HENSYN—Synthesis of heat exchanger networks

This program performs an algorithmic structure-synthesis for assigning a near optimal initial solution for a heat exchanger network problem. The program utilises the advantages of the Pinch-Point method of Linnhoff and Hindmarsch but without the originally manual procedure after assigning the pinch matches. For this purpose, the so-called Fast Algorithm of Pontin and Donaldson is modified and adapted, using the principle of "whole allowable heat load" instead of the original "Maximum possible heat load".

In the first step the program calculates the heat cascade of the problem, determines the minimum utility usage target and the pinch temperatures. The pinch temperatures locate the "bottlenecks" in a process design problem, which preclude further heat integration. The discovery of these bottlenecks can be used to alter the process design. In the second step the program creates a near optimal initial network having the features of the minimum utility usage and the probable fewest number of heat transfer units; furthermore, it makes an initial cost estimate prior to developing an actual network design.

PROGRAM COLSYN—Synthesis of distillation sequences

This program selects the optimal sequence of distillation columns for separating a multi-component mixture, when "simple sharp" separator units only are required, and neither products nor energy is recycled between separators. An ordinary two product distillation column which operates with high recovery of adjacent keys is an example of a simple sharp separation unit. The sequence cost is the sum of the separator costs, which combines the capital and operating expenses.

The problem of synthesising an optimal multi-component distillation system is solved by a combined decomposition and dynamic programming technique developed by Hendry and Hughes. First the separation sub-problems occuring in all possible separation sequences are generated, then the principle of optimality is used to select the optimal separation sequence.

STATCHAR: Statistical Characterization of Analytical Results

Authors: G. E. Veress, M. Kenderesy-Szucs
Dept. of General and Analytical Chemistry, Technical University of Budapest

To obtain the maximum information from experimental data it is necessary to characterise and know the magnitude of the errors involved, so that the accuracy and precision of the measurement is known, as is the bias and deviation of the mean of replicate experiments.

The programs in the STATCHAR package have been developed in an analytical chemistry department in order to obtain maximum information from experimental data. The programs go further than the simple mean and standard deviation calculation packages commonly available, since various statistical tests are performed to identify the magnitude of both the random and systematic errors. The ultimate reliability of any measurement method depends on the systematic and random errors.

3 programs are presented in this package:

CHAR for the statistical CHARACTERISATION of replicate measurements

COMP for the COMPARISON of sets of replicate measurements

CALIN for the statistical characterisation of a CALIBRATION LINE and of the measured result using this line.

Section CHAR can be used to characterise the precision and systematic error of measuring methods and is to give the statistical characterisation of the measured results of unknown material.

Section COMP performs the statistical comparison of two measured series, thus being suitable for comparing the precision and accuracy of measuring methods or giving the mathematical statistical comparison of the material under analysis.

Section CALIN performs the construction and statistical characterisation of the calibration line and the point and interval estimation of unknown material quantity using the calibration line.

The programs have been developed for extracting the maximum information from measured data. They are useful also in the teaching environment to demonstrate the statistical characterisation of measured data, and to link courses in statistical theory to the handling of laboratory data.

BATCHDIST: Batch Distillation Design Program

Authors: L. M. Rose, ETH Zurich

BATCHDIST is a program developed for the design of batch distillation systems. Emphasis is put on the design of the system as a whole rather than simply the simulation of a batch fraction. The batch column, condenser, boiler and control system are simulated over all the fractions making up the total distillation. The result is the total operating time for the distillation of the complete boiler contents. Total cumulative heat loads are also presented to enable better designs to be developed using economics to aid the selection.

Considerable efforts have been made to develop a design method which does not result in computer charges for the design which are out of all proportion to the final cost of the equipment being designed. Nevertheless, the method has developed to cover the majority of cases that arise industrially—including non-ideal, multicomponent systems with facilities for the decantation of one liquid phase when the condensate consists of two liquid phases.

The philosophy of the design method is to specify a batch distillation plant and to simulate its operation through the various distillation steps interactively. The interactive facility enables the kinds of processing decisions to be made during the simulation that might be made while operating real equipment. Sufficient information is given during the simulation for the bottlenecks to be identified and better equipment dimensions specified for the next trial. After working for a few hours with the program, a batch distillation system can be dimensioned with confidence.

Batch distillation is an excellent vehicle for teaching design to advanced students because of the large number of inter-related design variables that any multi-component batch distillation system contains. It is also a subject grossly neglected in many distillation courses, although the process is of significant importance in industry.

DISTILLATION DESIGN IN PRACTICE

by L. M. Rose
Technisch-Chemisches Laboratorium,
Eidgenossische Technische Hochschule
Zurich, Switzerland

Fields of interest:

Plant Design & Management; Process Design; Computers & Education; Performance Evaluation, Simulation, Modelling

COMPUTER-AIDED CHEMICAL ENGINEERING, 1

1985 xiv + 308 pages
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Approximate Month of Publication: August 1985

All industrial distillation design of any consequence is now done using computer methods. Though the fundamental principles still hold and must be taught, the students must also be introduced to these new methods, shown the principles behind them, and how to use them more effectively and intelligently.

This book is designed for use in a senior course in distillation design for the last undergraduate year or at postgraduate level. It is particularly useful for such a course because it integrates various disciplines (thermodynamics, design, control and distillation) that the student will have met separately in an earlier part of his course. The chapter headings given below show the range of topics treated. Whereas most senior books on distillation concentrate on solution methods for the algebraic equations defining the separation in the column, this book concentrates on those areas which are the real concern of the distillation equipment designer.

The text provides a link between the theory of distillation and industrial practice. Industrial state-of-the-art distillation design is concerned with multi-component distillation and computer methods for their solution. Hence the book concentrates on computer solutions, i.e. how to use distillation packages and how to interpret the results. Sufficient computer exercises are presented to allow them to be used for a "CAD Workshop" type course, with 50% of the course time being hands-on computer design of distillation systems. The appendix contains the program manuals and the source of all the necessary computer programs.

CONTENTS: Chapter 1. Design. 2. Vapour/Liquid Equilibria Data. 3. Binary Distillation. 4. Mulicomponent Distillation. 5. Batch Distillation. 6. Distillation Systems. 7. Column Internals. 8. Safety and Control. 9. Pilot Experiments and Debottlenecking. Nomenclature. Appendices: 1. Some useful conversions to SI units. 2. Some physical property data. 3. CAD exercises. 4. Computer program user manuals. Subject Index.

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Foundations of Computer-Aided Process Design

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