CACHE NEWS

News About Computers In Chemical Engineering Education.

No. 18

April 1984

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. After July 1, 1984, 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 above address. Contributions from CACHE Representatives are welcome. This issue was edited by J. D. Seader with contributions from a number of CACHE members and representatives. The next issue will be edited by D. M. Himmelblau of the University of Texas at Austin.

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NEW CACHE ACADEMIC TRUSTEE

At the November 3-5, 1983 meeting of the CACHE trustees, **Professor Ignacio E. Grossmann of Carnegie-Mellon University** was elected as an academic trustee. Dr. Grossmann was born in Mexico City on November 12, 1949. He received his B.S. degree in Chemical Engineering from Universidad Iberoamericana, Mexico City, and his M.S. and PhD degrees from Imperial College in London, where he worked under the supervision of Professor Roger Sargent. After obtaining his Ph.D. degree in 1977, he worked for one year at the Instituto Mexicano del Petroleo where he was in charge of the Process Optimization Group. He joined Carnegie-Mellon University in February, 1979, where he is currently Associate Professor of Chemical Engineering and a member of the Design Research Center.

Dr. Grossmann has over 20 publications in the areas of process flexibility, process optimization, process synthesis, and phase and chemical equilibrium. He is currently vice-chairman of Area 10C, Computers in Management and Information Processing, of the CAST Division of AIChE. His main research interests are in the areas of process flexibility and process synthesis. His work in the former area involves the development of analysis and optimization procedures that take into account variations and uncertainties in the design of chemical processes. In the area of process synthesis, his work involves the development of synthesis techniques that are based on mixed-integer programming. He is also developing design case studies for undergraduate education.

CACHE REPRESENTATIVES' RECEPTION

In conjuction with the AIChE Diamond Jubilee Annual Meeting in Washington, DC, CACHE held a reception for all CACHE representatives at the Washington Hilton Hotel. For the reception, Peter Rony organized a poster session on "The Selection of a Personal Computer for Undergraduate Engineers," and Monsanto Company officially presented FLOWTRAN to CACHE for use on department computers. The status of the FLOWTRAN project was presented and is described in detail on page 6 of this newsletter.

In the poster session, faculty representatives from several different chemical engineering departments discussed the decision process behind their university's requirement that all freshmen engineering students purchase a specific model of personal computer. The following are abstracts of the information presented in the poster sessions.

David E. Clough, "The Personal Computer System at the University of Colorado"

The University of Colorado is taking a different approach with regard to microcomputer acquisition and use. Via a campus-wide program at Boulder, several hundred IBM personal computers are being distributed to faculty to increase their computer literacy and to promote creative uses of computing. The College of Engineering & Applied Science is planning a phased program for student acquisition and use of microcomputers that builds on the faculty program already in place. Faculty preparedness and planned curriculum integration are key ingredients in the student program. The legal constraints associated with a state institution, such as the University of Colorado, carrying out both a faculty and a student program, have provided obstacles to implementation.

Mark E. Davis, "The Personal Computer System at Virginia Polytechnic Institute and State University"

The nineteenth century brought us an industrial revolution; the twentieth, the computer revolution. We move from the amplification and replacement of muscle power to the amplification and liberation of brain power. An IBM personal computer for every student thrusts the College of Engineering at Virginia Polytechnic Institute & State University to the forefront of this new revolution. All aspects of the events leading to the plans to require IBM personal computers and the implementation plans are described. If a certain announcement is made prior to the poster session, it could be a very exciting evening.

Complete details on the IBM PC program at Virginia Polytechnic are available from Professor Davis, Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061

Donald H. Sebastian, "Chemical Engineering Applications with Personal Computers at Stevens Institute of Technology"

The Chemical Engineering Department at Stevens Institute of Technology is in the midst of a curricular development program that aims to take full advantage of the capabilities of today's computer and graphics hardware. The approach, which relies heavily upon high-speed process simulation coupled to interactive alphanumeric and graphics displays to establish the connection between process fundamentals and process behavior, motivated specific choices in computer equipment.

We do not believe that the ready availability of inexpensive personal computers addresses the needs we perceive in Chemical Engineering education. Rather than adapting our educational program to the tool (the PC), we sought a tool that could be adapted to our program. This philosophy was shared by a number of engineering departments at Stevens and was a primary driving force in the selection of Digital Equipment Corporation's Professionals as the personal computer required of all entering freshmen as of September 1983.

Specifically, we see the DEC Professional as the only currently available personal computer with minicomputer rather than microcomputer capabilities. The ability to network the Professional to powerful mainframe computers and to share the various modular activities of our applications programs between processors significantly magnifies the power of either component. In this role as an engineer's workstation, the personal computer can be harnessed to serve student and professional alike.

Robert Cole, "The Personal Computer System at Clarkson College"

This fall, 650 engineering freshmen at Clarkson College each received a Zenith Z100 personal computer for use during their undergraduate years. We shall present the reasons for selecting the Zenith and our experiences with its use. A video tape presentation will show the distribution of 700+ computers, a short talk by Robert Plane, President of Clarkson College, and a short talk by Dave Bray, Dean of Computing.

LONG-RANGE PLANNING TASK FORCE ON MICROCOMPUTERS

CACHE has formed a task force, under the direction of Professor Stanley I. Sandler of the University of Delaware, to develop recommendations to the Long-Range Planning Committee of CACHE in the area of microcomputer usage. The main focus will be on the use of microcomputers in the standard curriculum areas (fluid mechanics, thermodynamics, kinetics, separations processes, control, design, etc.). This task force will consider the development and/or distribution of course materials and software within existing delivery systems. The software may be either of the calculational or computer-assisted instruction type. The goal of the task force is to suggest ways to distribute inexpensive quality software (including that commercially available) that contributes to undergraduate education in the standard curriculum areas. Such areas as computer graphics, data-base management, etc., will be considered only to the extent that they relate to the standard chemical engineering curriculum areas.

At a meeting of this task force on January 20, 1984, plans were made for an experimental electronic mail system using the University of Michigan Terminal System (MTS) via the Telenet and MERIT networks. The Telenet network can be accessed by local telephone calls on both 110-300 bps and 1200-bps numbers in 238 cities in the United States.

On May 9, one member of the task force accessed the electronic mail system and retrieved the following message left by another member of the task force:

"Just a note to let you know that I am now a Macintosh owner. I haven't done much with it so far, as only two programs (Macpaint and Macwrite) are available. First impression: Macpaint is superb; Macwrite isn't much of a word processor. The machine is painfully SLOW in doing almost anything with the current software and configuration. Comments: 1) More memory needed badly (supposedly a 512K version will be available soon). 2) One floppy is a big pain in the neck; the machine definitely needs another floppy or preferably a hard disk. 3) The mouse is handy, and icons are easy to understand; but the whole thing can become too 'cute' to deal with (e.g., it is far easier to erase a file with an ERASE command in PC DOS than it is to drag files to a wastebasket, empty the trash, etc.). This is particularly true for word processing, where one spends more time with a hand on the mouse than on the keyboard.

The unit itself is very compact and attractive. The Macpaint program is almost worth the price of the machine all by itself. Make a trip to the computer store to see a demonstration of this program. I'll keep you informed about my 'progress' with the Mac."

Electronic mail is discussed in an article starting on page 58 in the March 1984 issue of **Computers and Electronics.**

LABORATORY REACTOR SIMULATION PROGRAM

by H. Scott Fogler
University of Michigan

A laboratory reactor simulation program has been developed at the University of Michigan for the IBM-PC. The following is just a portion of an example session.

Example Run of the Guided Design Module
Part I
Laboratory Reactor Simulation

When the student first signs onto the guided design module, he/she is asked for his/her name and student ID number as such

> Please type in your name Eric Ye
> And your student ID number (Do not include dashes ie. 1193670482)1193670482

After the student has inserted the name and ID number, the module welcomes the student and then presents the main menu, shown below:

GUIDED DESIGN MENU

1) INTRODUCTION
2) LABORATORY REACTOR EXPERIMENTS
3) INDUSTRIAL REACTOR DESIGN AND PRELIMINARY RUNS
4) SIGNOFF

Which selection would you like to see?

If the student elects to see the introduction, this is what he/she would see:

Eric Ye this is the isomerization reaction

A --------> B

It is a gas reaction, carried out by passing A over an alumina catalyst. You are to determine the kinetics of the reaction and design an industrial reactor to produce the product B.

Press return to continue.

As in all industrial processes, the industrial reactor must be economical to use, thus look for the cheapest method possible to produce the product B.

The program is broken down into 2 basic parts.

In the laboratory reactor section you'll be given a budget of 5000 dollars and the option to build and use several laboratory reactors, whose inlet conditions you may vary according to your wishes.

Each of the several laboratory reactors will cost a different sum of money to build and run according to its complexity. You should have more than enough money to determine the kinetics of the reaction.

If you exhaust your budget, well, tough luck.

After you have determined the kinetics of the

reaction, you should proceed to the industrial reactor design section.

There you will be given the specifications of several industrial reactors available to you. Once you have determined which reactor best fits your needs, you should calculate the inlet conditions and the weight of catalyst you will use.

Press return to go back to main menu.

If the student chooses to see the second choice on the menu, laboratory reactor experiments, then a second menu is presented:

LABORATORY REACTOR MENU

1) INTRODUCTION
2) DESCRIPTION OF LABORATORY REACTORS
3) SELECT PHYSICAL AND THEMODYNAMIC PROPERTIES OF REACTANTS AND PRODUCTS
4) LABORATORY REACTOR RUNS
5) PLOT AND ANALYZE DATA
6) RETURN TO MAIN MENU

What section would you like to see (1-6)?

The introduction simply introduces the student to what reactors are available for determining the kinetics and what reactor parameters can be varied as shown below.

This section is designed to simulate the laboratory reactor runs that a chemical engineer would use to determine the kinetics of a particular reaction.

Press return to continue.

These are the laboratory reactors available to you

-DIFFERENTIAL REACTOR
-CSTR(slurry fed reactor)
-CARBERRY REACTOR
-TUBULAR OR PLUG FLOW REACTOR
-STRAIGHT THROUGH TRANSPORT REACTOR
-STRAIGHT THROUGH TRANSPORT REACTOR WITH HIGH RECYCLE RATE
-BATCH REACTOR

The conditions you may be able to vary are

-INLET FEED RATE
-INLET CONCENTRATION (varied by using an inert gas)
-INLET TEMPERATURE
-CATALYST WEIGHT

All the laboratory reactors operate adiabatically, i.e.: There is no heat loss or gain from the reactor (Q=0).

It is strongly recommended that before the laboratory runs are started, you look at the descriptions of each laboratory reactor and then select physical and thermodynamic properties of the reactants and products.

A final word of advice: No one reactor is the "ideal" reactor. Depending on the reaction, one may mask a part of the kinetics which another wouldn't; thus in order to get accurate kinetic data, you should use at least 2 or 3 different types of reactors.

Press return to go back to menu.

The select physical and thermodynamic properties available to the student are

The following data on the properties of the reactants and products will soon follow. It would be a wise idea to copy them down in your guide book.

The molecular weight of A and B is 60.15
The density of A and B is at 1 atm and 300 (K)=0.002443 g/cm^3
The catalyst available to you comes in spherical 2.00 mm diameter pellets
The catalyst density is 1.2 g/cm^3
The void fraction of packed catalyst bed=0.3
The dew point of A is 270 degrees Kelvin
The dew point of B is 253 degrees Kelvin
The heat capacity of A=20 cal/gmole K
Heat capacity of B=20 cal/gmole K
The heat of reaction is -1200 cal/gmole
All the laboratory reactors have an upper temperature limit of 1000 degrees K and operate at 1 atm pressure. Pressure drops across the reactor may be assumed negligible.

Press return to go back to the menu.

Further information on this program can be obtained by contacting:

Professor H. Scott Fogler
Department of Chemical Engineering
University of Michigan
Herbert H. Dow Bldg
Ann Arbor, MI 48109

PROGRAMS FOR PCs

by Bruce A. Finlayson
University of Washington

Two thermo programs are nearly complete. The database program, THERMOD, is now being tested in class use. It consists of data on thermodynamic parameters for a selected list of 93 chemicals, with provisions for the user to add to the list. The properties available are: molecular weight, normal freezing and boiling temperatures, heat of vaporization at normal conditions, critical temperature, pressure, specific volume and compressibility, acentric factor, dipole moment, solubility parameter, liquid density and its reference temperature, heat capacity constants, standard enthalpy of formation, Gibbs free energy of formation, constants in a viscosity correlation with temperature, Antoine constants and their temperature limits. The programs being tested are only able to retrieve this information, but the calculation program (still under development) will use those parameters to perform thermodynamic calculations. The THERMOD program is running on the Apple II+ and IBM PC, and the THERMOC program is running on the Apple II+.

The THERMOC program, currently only running on the Apple II+, will make the following calculations: compressibility factor, enthalpy, bubble and dew point (either pressure or temperature), and isothermal flash. In addition, it will display information on activity coefficients for a binary mixture and the vapor pressure versus temperature. The only part not yet programmed is to display the vapor-liquid phase diagram for a binary mixture. The type of thermodynamic assumptions included

are: ideal gas, Redlich-Kwong or Soave-Redlich-Kwong, pure component fugacity coefficients using RK or SRK or Poynting correction or Chao-Seader-Grayson-Streed, and activity coefficients using ideal solutions or regular solutions (solubility parameters) or Wilson equations (user-supplied data) or Van Laar equations (user-supplied data). The programs are written so that the student can easily test the adequacy of the choices in thermodynamic correlations. Not available yet are plotting routines for the results. Contact:

Professor Bruce A. Finlayson
Department of Chemical Engineering
University of Washington
Seattle, WA 98195

CACHE MICROCOMPUTER NOTES

Edited by Peter Rony

"Heart Cut," a popular department in **Chemtech** (a monthly magazine published by the American Chemical Society), consists of a series of brief notes and announcements on a wide variety of topics of interest to industrial chemists. As one step towards enhancing the value of CACHE NEWS as a vehicle for disseminating timely information on computers, we introduce in this issue "CACHE Microcomputer Notes." If you have microcomputer news items that you feel would be of interest to faculty, please write them in the style given below (or in **Chemtech**) and send them to Peter Rony (Virginia Polytechnic Institute, Blacksburg, VA 24061).

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Faculty are often placed in the position of tailoring or modifying microcomputer machine code software for their own laboratory needs. The March 8, 1984, issue of **EDN** (Cahners Publishing Co., 221 Columbus Avenue, Boston, MA 02116), pp 65-76, summarizes cross assemblers for a wide variety of 8- and 16-bit target microprocessors. Most of the cross assemblers operate on a host equipped with either the CP/M or MS-DOS operating systems. Target microprocessors include the TMS100, COSMAC/1802, 1805/1805A, TMS320, F8/3870, COPS400, 6502, 6800, 6801, 6805, 6809, TMS 7000, NEC 7500 and 7800 series, 8048 and 8051 families, 8085, NCS800, Z8, Z80, 8086/8088, Z8001/Z8002, 9900, 9995, 16032, and 68000.

The March 8, 1984, issue of **EDN**, pp 132-170, also contains an article on "Personal-Computer Add-Ons and Add-Ins"; namely, boards and peripherals that convert a personal computer into a laboratory instrument or engineering aid. Using such products, one can configure personal computers for data acquisition, measurement and control, analog signal measurement and analysis, IEEE-488 interfacing and control, microprocessor development, semiconductor device programming, voice I/O capability, and so forth. The products and addresses of 165 different companies are represented, and a reader service card is provided. The personal computer add-ons/add-ins summarized in the table are subdivided into the following categories:

A = Apple
B = IBM PC
C = Commodore
S = S-100 Bus
T = TRS-80
H/Z = Heath/Zenith H/Z-89
I/E = IEEE 488/I/O
RS-232 = Standard serial interface

A frustrating experience encountered by novices and professionals alike occurs during the attempt to communicate between brand-X personal computer and brand-Y printer using brand-Z printer software. "Standard" RS-232C serial connections are made between the computer and printer; but when the big moment arrives to test the combination, the printer remains silent. The problem is that RS-232C is not an effective standard, Manufacturers select different pins and different logic levels to achieve handshaking capability, and one is always forced to refer to manuals for details on the wiring of the RS-232C connector pins. A new book, **RS-232 Made Easy: Connecting Computers, Printers, Terminals, and Modems**, by Martin D. Seyer (Prentice-Hall, $18.95), provides a good introduction to RS-232C. Half the book consists of the following appendices, which are most useful:

Appendix A. EIA Standard RS-232C
Appendix B. EIA Standard RS-449
Appendix C. Industrial Electronics Bulletin No. 12
Appendix D. RS-232 Circuit Summary with CCITT Equivalents
Appendix E. Tools of the Trade
Appendix F. RS-232 Pin Assignments for Computers and Peripherals
Appendix G. Interconnections Between Computers and Peripherals
Appendix H. Interface Problems and Remedies

As a test, the editor determined whether the following personal computers and peripherals were mentioned in Appendix F: Heath/Zenith Z-89 serial ports (yes), Micro Peripherals Inc. MP1-88G or MP1-99G dot matrix printers (no), and IBM PC (yes).

BYTE magazine, in a November 1983 issue that is dedicated to the IBM PC, contains the article, "Expanding the IBM PC," which uses extensive tables to survey PC expansion boards in seventeen categories: Z80 coprocessors, memory, disk-drive controllers, multiple interfaces, advanced graphics, parallel I/O, clocks, print-spoolers, prototyping, speech synthesizers, EPROM and EEPROM programmers, extenders, serial I/O, multifunction with and without memory, integral modems, and miscellaneous.

The evaluation of laboratory reports is difficult in the large classes that characterize engineering colleges at state universities. AT&T software entitled "UNIX Writer's Workbench" (Western Electric Software, Sales and Marketing, P.O. Box 25000, Greensboro, NC 27420, [919] 697-6530) is being tested as a productivity tool in English classes. An IBM PC-UNIX can be used. Details on this software are discussed in a recent article, "The UNIX Writer's Workbench Software," that appears in the October issue of **BYTE** magazine. In its current form or as a forerunner to more sophisticated software, a writer's workbench promises to be a significant contributor to the improvement of

undergraduate communications skills. Some of the capabilities of the AT&T software are illustrated by the following command-function table:

abst file	Evaluates text abstractness
acro file	Finds acronyms
findbe file	Identifies difficult syntax
org file	Shows text structure
parts file	Assigns grammatical parts of speech
sexist file	Finds sexist phrases and suggests changes
style file	Summarizes stylistic features
syl -n file	Prints words of n syllables or longer
topic file	Provides clue to topic, keywords
wwb file	Runs proofreading and stylistic analysis
proofr file	Runs proofreading and stylistic analysis; finds split infinitives
diction file	Finds awkward phrases and suggests changes
double file	Detects repeated typings of words
punct file	Checks punctuation
spellwwb file	Checks spelling using spelldict
prose file	Gives extended editorial comments

MICROCACHE PROJECT

by Brice Carnahan

The purposes of this project, under the direction of Professors Brice Carnahan and H. Scott Fogler, are to:

1. Develop prototype micrcomputer-based software for delivering educational materials and programs (modules) for chemical engineers and engineering students.
2. Prepare several educational modules to test the software.

During the past several months, the MicroCACHE supervisory system and utility programs have been rewritten and improved so that they can be executed on the IBM Personal Computer. The machine configuration for which the software has been designed is:

IBM PC or PC/XT with:
(1) two double-sided, double-density floppy disk drives or one floppy-disk drive and one hard-disk drive
(2) 256K fast memory
(3) color/graphics adapter
(4) monitor (mono or color)
(5) 8087 coprocessor chip (optional)
(6) matrix printer (optional)
(7) PC DOS 2.0 operating system

The MicroCACHE software was originally implemented on the basic Apple II+ microcomputer, which, given its limitations (small memory and disk storage, 40-column screen, uppercase-only alphabet, etc.), can only handle relatively small educational modules. Since there is interest in the possibility of developing "large" modules, involving, for example, many bitmapped graphics screen pages and sizeable, computationally intensive object programs such as would be needed for process design and simulation, it was felt important to convert the software for execution on larger, more capable machine.

At this point, well-configured IBM PC and PC/XT computers appear to be the best choice from the standpoint of widespread availability and the presence of many "compatible" machines on the market. The software in its present form will run successfully under PC DOS 1.1 on a 128K machine without a coprocessor. However, some DOS 2.0 features will be used in the future to allow for the possibility of larger modules (hence the larger memory). The color/graphics board is essential since the computer cannot handle bitmapped graphics without it.

The use of the coprocessor is suggested since experience with compiled object programs that involve mostly floating-point calculations, and little input/output indicates that execution time can be reduced by factors of from five to twelve.

Five manuals for the IBM version have been written and edited and put into machine-readable form and will be available for distribution by May 1:

1) **MicroCACHE User's Manual:** This is an introduction to the MicroCACHE System, intended for use by students who have not used the software before.

2) **MicroCACHE Instructor's Manual:** This is an introduction to MicroCACHE for the instructor and covers, in particular, recovery of user-related information (e.g., history of module use, responses to examination, and evaluation questions).

3) **MicroCACHE Module Writer's Manual:** This is a detailed manual describing how to modify existing modules (e.g., change examination questions, reformat screen displays, modify menu selections, etc.) and how to create a new module from scratch.

4) **MicroCACHE Graphics Package Manual:** This manual describes the preparation of graphical screen frames (either independently or as part of a running object program) using our graphics package.

5) **MicroCACHE System Overview:** This manual describes the system from the standpoint of software organization and data structure.

A few of the educational modules are now being considered for use on the IBM/PC; perhaps ten will be available by the end of the summer.

Professor Carnahan and Chris Jaeger, one of his students, will be describing the current MicroCACHE software in the session on Microcomputers in Education at the AIChE meeting in Anaheim on May 23 (Session 41).

A distribution mechanism for the software and available modules will be established before the beginning of the fall term, 1984.

More information can be obtained by writing to

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Dept of Chemical Engineering
University of Michigan
Dow Bldg, North Campus
Ann Arbor, MI 48109

FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

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 currently supervising the preparation of load modules for a wide variety of main-frame-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. **Amdahl** computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).
2. **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).
3. **IBM** and IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and 43XX with the VS FORTRAN compiler (Program #5748-F03) running under the VM/CMS operating system (9-track, 1600 BPI tape).
4. **IBM** and IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and larger 43XX with the FORTRAN IV H extended compiler (Program #5734-F03 plus the library) running under the OS1/MVS operating system (9-track, 1600 BPI tape).
5. **DEC 20XX** mainframe computer running with the FORTRAN-20, Version 7 compiler (9-track, 1600 BPI tape).
6. **DEC VAX 11-7XX** series of super minicomputers running with the VMS operating system.

Conversions are also underway for the DEC 10, CDC, and Prime machines, as well as other IBM versions. Each 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. FLOWTRAN tapes have already been distributed to departments at the following universities:

Univ of Akron	McMaster Univ
Arizona State Univ	Michigan Tech
Brigham Young Univ	Univ of Michigan
Univ of British Columbia	Mississippi State
Bucknell Univ	Univ Nacional del Sur
UC - San Diego	(Argentina)
Case Western	Univ of Nebraska
Columbia Univ	New Jersey Inst Tech
Univ Concepcion (Chile)	CC-CUNY
Univ Connecticut	North Carolina State
Cooper Union	Northeastern Univ
Cornell Univ	Tech Univ of Nova Scotia
Univ Delaware	Univ of Pennsylvania
Drexel Univ	Pratt Inst
Ecole Poly	Rensselaer Poly Inst
Florida Inst Tech	Rice Univ
Georgia Tech	Rose-Hulman
Univ Houston	Rutgers
Howard Univ	Univ of Saskatechewan
Illinois Inst of Tech	Texas Tech
Univ Illinois @ Chicago	Univ of Utah
Iowa State	Univ of Washington
Kansas State	Wayne State Univ
Univ Southwestern Louisiana	
Louisiana State Univ	West Virginia Tech
Lowell Univ	Univ of Wisconsin
Univ of Massachusetts	Worcester Poly

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.

REPORT ON CHEMI PROJECT

by
David M. Himmelblau

Introduction

Advances in computer hardware as well as telecommunication systems technology in the 1970's contributed to the development of new techniques and systems for the education of scientists and engineers. The CHEMI project represents such an effort in the field of chemical engineering.

The first phase of the project, begun in 1975 via Grant No. HES-75-03911 from the National Science Foundation, resulted in the production of more than 300 single-topic, stand-alone instructional modules spanning the key subject areas in the undergraduate chemical engineering curriculum. Each module was approximately 20 pages, covering a subject content roughly equivalent to one contact hour of lecture. These modules were originally written for off-line study and are being published by the AIChE as the Modular Instruction Series, as described later in this newsletter.

In 1978, the second phase of the CHEMI project was initiated via National Science Foundation Grants Nos. SED-79-12021 and SED-81-16698. The major goals of the second phase were 1) to prepare modules in order to fill gaps in the originally proposed modular structure, 2) develop advanced-level modules, 3) prepare 500 abstracts of topics not included in the modular structure, 4) to test, revise, and update the modules that had been produced, 5) to develop a usage inducement system to encourage various groups of consumers to use the system, and, finally, 6) to seek out means to provide for continuing dissemination of the

modules. These aims, for the most part, have been met. Over 75 new modules have been added to the original modular structure. Eighty percent of the modules prepared in the first phase have been edited, revised, and updated. An on-line information system has been developed that will permit a user to access over 500 abstracts of key topics in the field of chemical engineering, and, eventually, 400 instructional modules covering the following subjects: **Material and Energy Balances, Thermodynamics, Transport Phenomena, Stagewise and Mass Transfer Processes, Process Control, Kinetics, and Design.**

In the original planning for the information system, a number of features were thought to be important to chemical engineers using micro and minicomputers:

1. Help in choosing modules for study
2. Abstracts of outside sources
3. Computer programs for chemical engineering calcuations
4. Glossary of terms and symbols
5. Interactive mastery testing
6. Record-keeping
7. Report generation
8. Curriculum path selection.

One of the major goals of Phase II of the CHEMI project was to develop a computer-aided instruction package that would offer all of the above features. However, because of the limitations of time and funds, the computer programs, interactive testing, and record-keeping features of the system have not been included at this time. The high cost of designing and coding the required software for the CHEMI information system prevented designing an interactive, computer-aided instruction program as elaborate as, for example, the PLATO system. The CHEMI on-line system focuses on information retrieval, primarily for searching, diagnostics, and reference. The system accesses the modules and abstracts through a keyword search of the index and/or sequence selection. A module, part of a module, or any screen of information can be printed off-line. A glossary of chemical engineering terms is available and can be searched by term or by notation symbol. The shortest path through a sequence of modules for a curriculum can also be obtained. By adding or deleting modules from a sequence, the user may build a tailor-made study sequence. To assist in this process, module abstracts, objectives, and prerequisites may be viewed.

The information system has been written in the "C" programming language and runs on a UNIX operating system. The choice of C as the language makes the source code highly portable between computers because C is a young language whose conventions have been standardized. The language is highly structured, which is desirable for good programming, and it is modular. The machine and operating-system routines are isolated, allowing a program to be easily expanded. As UNIX becomes more widely accepted as an operating system, the C language is gaining in popularity, especially on microcomputers.

In the preliminary planning of the project, in the later 1970's, we decided to design the CHEMI system to avoid hardware dependency typically found in NSF educational materials and make it truly portable. It was recognized that microcomputers and terminals would not be standardized among the many colleges and universities using computer-based educational materials thus preventing the widespread use of any information system that was dependent on hardware. Furthermore, hardware rapidly becomes obsolete. There was agreement also that hardcopy was just as important as retrieval on a CRT and that high-speed line printers were the only way that copies could be retrieved at minimal costs. Dot-matrix printers and character printers were far too slow for hardcopy output of 40 pages of modular material on demand.

Thus, in the planning stage of the project, it was thought that there would have to be two versions of the CHEMI information system: Version 1 for output on dumb terminals and line printers, and Version 2 for output on graphics terminals and printers.

In creating the data base for Version 1, because of certain limitations in the capabilities of standard ASCII terminals, we had to develop extensive guidelines for drawings and for equation formatting that set standards for Greek letters, subscripts and superscripts, and certain mathematical symbols. Examples are shown in CACHE News No. 17.

We have not produced Version 2 of the CHEMI system although we have employed the DEC GIGI system's graphics editor to enter some figures in the Materials and Energy Balance modules, as shown in CACHE News No. 17. We have found it costly to enter data using the graphics editor, and the software for some functions that we need is not yet available.

Salient Features of CHEMI ONLINE

From the user's point of view, some of the salient features of the CHEMI ONLINE system are:

1. **Direct access to information.**
   Very few instructions and screens are neeeded to get to the desired information; often screens can be bypassed altogether.

2. **Swift response time.**
   At a terminal baud rate of 2400 and with reasonable access to timesharing, the most time-consuming searches take less than three seconds. There is also keyboard type-ahead. This means that commands may be entered sequentially without having to wait for the screen to redraw and the cursor to appear.

3. **No computer sophistication required**
   The program is menu driven, has extensive files, displays prompting messages where needed, and emulates traditional library reference searches.

4. **ANYTIME availability**
   This allows leaving any part of the program at anytime, allows quick access from any one function to another, and prevents the user from getting lost.

5. **Input traps**
   Commands entered in incorrect format are either standardized internally or ignored and asked for again. Control keys and other nonprinting characters are ignored. The Delete or Rubout key, instead of immediately terminating the program, first asks for verification then resets the terminal settings altered by the program and then exits.

From the systems programmer's point of view, some of the salient features are:

1. **Expandable text files**
   Additional modules, abstracts, and index entries can be added by following the existing formats of the text files. The program is already set up to recognize user requests for all other modules beside the MEB's should they be added on.

2. **Structured programming**
   Modifiable, modular structured programming in "C" with well-documented source code and programmer's information sheet were prepared.

3. **Portability**
   As will be discussed below, the system is designed to be portable to various machines, operating systems, and terminal types.

Internal Characteristics

A view of the characteristics of the system helps evaluate portability and expandability. For the text display files, the main specifications are that of format. All lines are fewer than 66 columns; all screens are 20 lines or fewer. Text screens fit within the main program screen of 80 columns by 24 lines. Each module is written in a specified order, with each section marked by a specific symbol that the program recognizes. When properly formatted, each module is run through a small auxiliary program that appends a list of the line numbers indicating where each section starts. In effect this "thumbnotches" the modules for quicker run-time access.

The abstracts, index, glossary, and other texts fit within the same screen-size limitations. Their length is not critical, however; and they may be added to as external system memory permits. The index and glossary may have entries deleted, inserted, and appended without any effect on program performance. In fact, the design of the program itself is sufficiently independent of the contents of the text files it accesses that the program may be used with a variety of educational subjects if they could be presented in a similar way. To use the program in another area of science, such as geophysics, it would be necessary to develop modules and abstracts on the subject in the same specific format as the present system. An index of geophysical keywords and a glossary would be necessary; a list of module titles, a sequence of study paths, and modified help section would complete the system.

Portability

Storage of the Material & Energy Balance modules presently online takes up by far the largest portion of the system's memory requirements; namely, 1600 Kilobytes (K). The abstracts and all the other text files require 700 K. Auxiliary UNIX system files reside in 15 K. The program itself, both source and object code, take up 64 K. Storage of the total system on tape or disk would therefore require 2.4 Megabytes (MB). The object code, which incorporates the auxiliary system files once the source code is compiled, takes up only 39 K of memory. Thus even a microcomputer with limited internal memory could run CHEMI ONLINE as long as the external storage was sufficient.

CHEMI ONLINE is in principle portable to a wide variety of types of terminals. The program accomplishes this feature by accessing two specific UNIX files called "termcap" and "curses." "Termcap," a database, contains a description of the operations and capabilities of over 200 types of terminals. The following is an example of the specifications in the database for a Micro-Term Act-5a (a terminal commonly used in the project):

```
m5a|act5a|microterm act5a:
:am:bs:pt:ku=^Z;kd=^K;kl=^H:kr=^X:cl=^L:cm=^T%.%.:
:co#80:li#24:nd=^X:up=^Z:ho=^]:al=10*^A:dl=W"dc=^D:
:im=^S:ei=^G:uc=/EA:us=/EZ:ue=/E[:so=/EX:
:se=/EY:
```

Although most terminals that we believe might be used for CHEMI ONLINE are already included in "termcap," a systems programmer can enter a new terminal by describing all its operations and capabilities using the Termcap database conventions.

The name of the terminal being used is identified in the terminal environment, which is usually set automatically at login. In UNIX this step is accomplished in the login file with the statement "TERM=act5a; export TERM" (if "act5a" is to be the terminal). The user of CHEMI ONLINE should not have to be concerned with the terminal type.

The second file mentioned above, "curses," provides cursor and screen control commands that access the entry in "termcap" for the particular terminal being used.

The CHEMI ONLINE program does not drive a printer; it places online copies of requested material in a file called "chemout." This file can be printed by the user, after exiting CHEMI ONLINE, using commands specific to the local system. Thus the user can specify any necessary account number, password, remote site number, character conversion, etc., independently of the program. The only requirements of a printer, therefore, concern characters and format. It must be able to print all ASCII characters (32 to 126) and must print at least 65 columns.

The program runs on the 4.2 Berkeley version of UNIX; it is compatible with Version 7 of UNIX. The growing acceptance of UNIX within the educational and engineering community, the growing number of computers that are able to support UNIX, and the number of UNIX-like systems that have been produced for a wide variety of machines, all assure a wide range of portability for CHEMI ONLINE. Additional portability was assured by using the UNIX program "lint" during software development. This program checks C program code for word-size dependent constructions, undeclared pointer-returning functions, functions with a variable number of arguments, multiple definitions of variables, and other cases that could cause problems in some machines but not in others.

CHEMI ONLINE can be made portable to other operating systems as well. A limiting factor is the capability of the C compiler used. A little background will help clarify this idea. The C language was selected for the project because of its renowned portability. It is a relatively low-level language and as such has fast and direct control of the computer. By the same token, it lacks ready-made string manipulation, file access, buffered

input-output, and other functions expected of higher level langauges. These are provided by supporting files such as the standard I/O library. The extent and quality of the higher level routines thus supported are what make a big difference among the various C compilers.

Most compilers available on large operating systems may support the program as is; others may be lacking some functions that would need to be rewritten. Of course, C compilers in a UNIX package would support all necessary functions.

With either a UNIX system or an appropriate C compiler, the system can be transported to a microcomputer. The two major considerations for success are external storage and screen control. Floppy disks would be cumbersome to use and necessitate some rewriting of the software. A hard disk of 5 MB or more of external storage would be able to hold the entire CHEMI system. It could be downloaded onto the hard disk from a mainframe with the use of a modem and the microcomputer's terminal program. The screen control functions must then be taken into account since they would differ from one microcomputer to the other. There are two possibilities. One is to code in the screen control capabilities for the specific micro as an entry in the aforementioned "termcap." The other is to replace all "curses" functions in the program with the local screen-control functions. Either method would then allow the program to run on the particular microcomputer.

Alteration and Expansion of CHEMI ONLINE

The program also accesses two local files that a systems programmer may want to alter. One, "defs.c," defines all constants used in setting up the main screen and in accessing specific parts of some text files. The other, "filebox.c," defines the names of all the files used by the program. That is, external file names are given internal file names. Path names can be assigned to the files in order to set up certain directories to hold certain files; for instance, an abstracts directory. After the initial installation of the system, no maintenance should be necessary.

Possibilities for future alteration and expansion certainly exist. First of all, the remaining module groups could be added. Much of the indexing work for the Process Control, Thermodynamics, and Transport module sets has already been done and is included in the online index.

Systematic pre- and post-testing of the student as he/she progresses through the system remains a desirable feature for future addition. It should be noted, however, that a method of testing that is fair and comprehensive, that can analyze answers against a variety of possible responses, that can be made cheat-proof and be applicable to both undergraduate students and practicing professionals, is a sizable task and is of a different order than the kind of information retrieval that has been prepared so far.

Limitations of the System

References are made throughout the system to material that is not currently online. The articles to which the abstracts refer or the books mentioned as suggested reading, of course, should not be expected to be online. However, modules which are not online but are referenced by the index and the study sequences may frustrate the user. Obviously, the system will be most useful when the user can depend on it to cover all basic areas of chemical engineering.

The limitations concerning portability have already been mentioned; those remaining concern the terminal screen. It must be 20 x 24 inches unless the screen-position constants in the program are carefully altered. Subscripts and superscripts must be displayed on successive lower or upper lines, respectively. Some figures are drawn with the underline character, which is not universally terminal-supported. Greek letters and some mathematical symbols are spelled out, and mathematical equations are represented in a form suitable for terminal display. This form often differs from the printed form familiar to the user.

More information can be obtained by writing to:

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THE DOIG TROUBLESHOOTING PROGRAM

by David M. Himmelblau

Introduction

Troubleshooting problems are used in several schools (1-6) in the United States and overseas in connecton with instruction in chemical engineering. Most of these problems are used as part of senior design courses although some elective courses focus on troubleshooting exclusively. Various types of problems have been prepared for analysis often based on real industrial experiences. A problem might take up four or five hours of class time for individual effort with consulting and data provided by the instructor or teaching assistant. In addition, it is usually helpful to prepare the students for the sessions by a lecture and discussion on the strategy of troubleshooting (preferable for an industrial environment) including specific schemes to attack plant faults.

As to the types of problems used in troubleshooting, Woods (7) has spent considerable effort and developed a large set of cases at McMaster University. In the problem-based learning approach, instead of having lectures, students are given the problem and asked to solve the problem in a fixed period of time. Both problem-solving skills and learning skills are developed simultaneously. Various types of formats for the presentation of the troubleshooting problem exist. For example, one finds short written statements, written material, together with visual aids such as a movie or a taped interview of slides, computer simulations, or personal appearances by engineers serving as consultants. The written description is the cheapest and easiest to prepare for an instructor and the most common format for troubleshooting problems. Visual and audio components have been developed at McMaster University. The topic here is

the computer simulation, developed by Ian Doig (8) at the University of South Wales, for a complete chemical plant.

Learning Objectives

Doig's (8) program emphasizes learning problem-solving skills. Woods (7) has neatly summarized the key learning objectives for problem solving. Not all of the Wood's objectives can be accomplished in the session with Doig's problem, of course; but almost all can be employed over a period of time.

CACHE has cooperated with Professor Doig in making his troubleshooting and diagnostic code available to chemical engineers. His program is the first to make substantial use of computer-student interaction in process fault diagnosis. Most attempts to engage in the improvement of skills in troubleshooting have let students work on their own to determine the cause of the fault(s) in the process or work via groups; but the students obtain information from the instructor by asking questions about past experiences, the results of their calculations, the results of experiments, etc. Also, usually the troubleshooting cases that are examined refer to single pieces of equipment or small collections of equipment. Often the emphasis is placed on students to work on developing a suitable strategy for solving the problem, and little effort goes into an actual solution of the problem that is realistic.

Process Diagnostic Exercises

The process diagnostic exercises prepared by Doig 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 (vapor) phases to resolve the cause (or causes) of a discerned malfunction (or distinct drift from normal, a desired behavior) in a chemical plant. The exercises imitate functions to be carried out by process designers and those engaged in operating a typical chemical plant. They cause a student to bring to bear many of the skills he or she has separately acquired in other courses in tackling a common chemical engineering problem. Emphasis is based on:

1. **Identifying the problem** correctly without basis.
2. **Postulating cogent causes** and assembling pertinent knowledge and information.
3. **Devising tests** which can confirm or deny the postulated cases.
4. **Carrying out the tests.**
5. **Analyzing the results**; then postulating other causes and conducting further tests as required.

If tests confirm a particular postulated cause with an economically acceptable measure of confidence, the student is asked to apply the appropriate remedy and verify the diagnosis.

The exercises are concerned with the performance of a hydrocarbon chlorination plant with feedstreams:

- Hydrocarbon (whose properties are fictitious and lie between those of benzene and toluene)
- Chlorine
- Water

The plant products are:

Unreacted hydrocarbon
Hydrocarbon monochloride
Hydrocarbon dichloride
Aqueous hydrochloric acid

Two distinct parts (or plant batteries) exist for the process--the SYSCHEM plant and the DISTILLATION plant. The SYSCHEM plant which produces 1) the aqueous hydrochloric acid and 2) the unreacted hydrocarbon, hydrocarbon monochloride, and hydrocarbon dichloride as a mixed liquid stream which is fed in the second part (or battery) to the DISTILLATION plant. The latter consists of two fractional distillation columns in series. This plant separates the mixed liquid feed stream into a 99 mole% pure HC2 product, a 95 mole% pure HC product, and an 88 mole% pure hydrocarbon product, which becomes recycled to the SYSCHEM plant. Figure 1 shows the SYSCHEM plant; the distillation plant was shown in CACHE News No. 17.

What Professor Doig has accomplished is to set up a large data base of information that represents a flowsheet for a chemical plant based on plant simulations so that the plant does not have to be simulated to produce measurements. Data are made available on demand for measurements at a large number of locations in the plant for streams such as cooling water, steam, chilled water, and other utilities. In addition, measurements can be solicited as requested by the user on all the details of valves, pumps, blowers, and so forth, as well as physical data for all components of all streams. Another feature of the system that provides a realistic representation of a plant is a randomly generated Gaussian distributed error that is contained in all the measured values reported.

A student is provided with plant manuals for both the SYSCHEM and DISTILLATION plants. These contain all the information required to begin solving the diagnostic problems set and instructions for obtaining the various measurements at various points in the process needed to complete the diagnosis. One starts by obtaining a set of routinely logged plant measurements to allow a student to discern that a problem exists and to define it and to develop a diagnosis. All other (nonroutine) measurements incur a dollar cost charge and a charge as well for the "off-specification" product produced while those measurements are being made. A skilled diagnostician will determine via correct logic the true cause of the fault set for him or her to solve and yielding an approximate "par value" (in dollar charges accumulated) for each particular fault exercise set. None of the fault exercises are of equal difficulty, and no two fault exercises are likely to have the same par value. An instructor should be more interested in following the logic demonstrated in diagnosis so that the dollar charges will serve only as a guide to whether the diagnosis was prudent and rational or a series of (often expensive but occasionally lucky) gambles. Malfunctions that can be introduced include leaks, impurities, off-specification compositions, restrictions on proper flow rates, and excessive use of utilities.

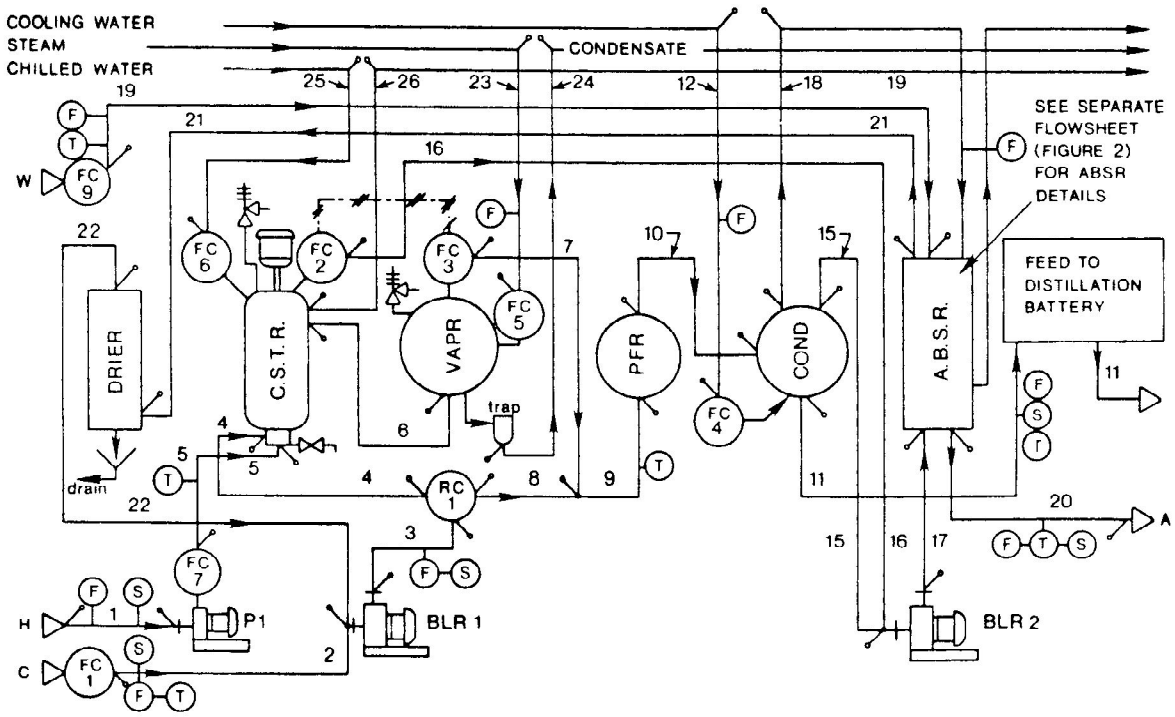

Figure 1. Flowsheet for Revised SYSCHEM Plant

Professor Doig recommends (**Chemical Engineering Education,** Summer 1980, p. 130) that no more than 10 students be allocated per instructor if the whole class works on a common problem. He also suggests that real plant experience helps provide the proper type of responses to student questions.

CACHE has exerted considerable effort to make the computer code portable. The code has run on 1) CDC Cyber 170/750, 2) CDC-600, 3) IBM-370/158, 4) VAX 11/780, and 5) DEC 20 computers. Comment statements explain the (few) changes needed to make the code compatible with one of the above computers. Coding of the program is in standard FORTRAN IV (1966), but some special features of your FORTRAN compiler may cause errors to be cited in compiling. CACHE does not support the program. CACHE would appreciate comments about education benefits and experiences using the code. If you are interested in obtaining the program on a tape, contact:

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INTEGRATION OF COMPUTER USAGE INTO UNDERGRADUATE CURRICULUM

CACHE has established a committee, under the direction of Professor Morton M. Denn of the University of California at Berkeley, to study possible ways in which CACHE can assist chemical engineering departments in integrating computer usage into the undergraduate curriculum, particularly the core courses. CACHE recognizes that many departments are currently undertaking studies of this subject. If any department has prepared any working documents for use within its own department, CACHE would very much appreciate receiving copies in order to assist in evaluating the current status of computer usage and future plans. Any comments that are not included in formal reports would, of course, be welcome. Any department that has not already submitted such material to Professor Denn at the following address is encouraged to do so:

Professor Morton M. Denn
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Berkeley, CA 94720

1985 ICHEME - CAMBRIDGE CONFERENCE THE USE OF COMPUTERS IN CHEMICAL ENGINEERING

March 31 - April 3, 1985 - Cambridge, England

Organized by the Institution of Chemical Engineers on behalf of the European Federation of Chemical Engineering.

CALL FOR PAPERS

The Institution of Chemical Engineers (Rugby, England) is calling for papers for a conference on "The Use of Computers in Chemical Engineering" to be held at Robinson College, Cambridge, UK. This will continue a successful series of symposia held at the invitation of the EFCE Working Party on Computer Applications, taking place in Montreux in 1979, Heviz 1980, Vienna 1981, Antwerp 1982, and Paris in 1982.

In 1985 the emphasis throughout will be on the presentation of new information on either technology or its applications. Papers describing applications will be encouraged, especially if they contain detailed information relating to the value of the study, estimated savings, etc. Papers describing new work in other areas of process CAD will be considered for inclusion. A "poster session" is planned where authors can present their latest ideas, which may not have reached a stage which justifies a full paper.

Proposed Themes For Conference

Operability Considerations at the Design Stage
- process dynamics
- hazard & operability studies
- fault trees
- availability & reliability
- measures of controllability
- flexibility/resilience

The Design of Flowsheets
- new flowsheeting technology
- batch & semi-batch processes
- multiphase systems
- synthesis of whole flowsheets
- costing and economic analysis

The Influence of New CAD Technology
- databases & databanks
- graphics
- integraton of systems
- new hardware (e.g. micros & local area networks)

Aids for Plant Operation
- monitoring & analysis of plant performance
- fault detection/diagnosis
- reconciliation of measured plant data

The Management of Design
- useability of design systems
- issues of liability & responsibility
- uncertainty & risk

Provisional Timetable for Authors

Early 1984	Final Call for Papers
August 1984	Deadline for abstracts
November 1984	Draft of final paper
January 1985	Final paper for printing

Plenary sessions are planned, each major session conducted by a Chairman-Rapporteur and will include 4 or 5 papers of 30 minutes each (including discussion). It is intended to publish the conference proceedings in the IChemE's Symposium Series. Besides the proposed Poster Sessions, there will be opportunity for discussion in rooms set aside for informal gatherings. An exhibition of software/hardware relevant to the theme of the Conference will run concurrently.

Offers of papers, comments, or suggestions should be directed initially to:

F. A. Perris
Engineering & Scientific Systems Department
Air Products Limited
Hersham Place
Molesey Road
Walton-on-Thames
Surrey KT12 4RZ
ENGLAND
Tel: 09322 49337 Telex: 917243

Further information can also be obtained from: The Conference Section, The Institution of Chemical Engineers, 165-171 Railway Terrace, Rugby CV21 3HQ ENGLAND. Tel: 0788-78214 Telex: 311780

MATHEMATICAL SOFTWARE

by William E. Schiesser

DPDES: An IMSL Routine for Partial Differential Equations

The modeling of chemical engineering systems frequently leads to systems of partial differential equations (PDEs). For example, if the problem system has at least one significant spatial dimension, e.g., axial distance along a heat exchanger or tubular reactor and the time-dependent behavior of the system is of interest, then at least two independent variables, space and time, must be considered, and thus PDEs are required to model the system.

The solution of PDEs is one of the most demanding problems in applied numerical analysis. Recently, computer routines have begun to appear that facilitate the numerical integration of PDE systems. One such routine, DPDES, available in the IMSL (International Mathematics and Statistics Library* is described here.

DPDES can accommodate systems of PDEs of the form:

$$\underline{u}_t = \underline{f}(x,t,\underline{u}_x,\underline{u}_{xx}) \qquad (1)$$

where $\underline{u}$ is a vector of dependent variables, t is an initial-value independent variable, e.g., time, $\underline{x}$ is a boundary-value independent variable, e.g., axial position, $\underline{f}$ is a vector of user-defined functions, and a subscript denotes a partial derivative, e.g., $\underline{u}_t$ is the partial derivative of $\underline{u}$ with respect to t. Clearly equation (1) encompasses a broad spectrum of one-dimensional PDEs, but some limitations are given in the subsequent discussion.

The boundary conditions for Equation (1) accommodated by DPDES are:

$$\underline{a}_1\underline{u} + \underline{a}_2\underline{u}_x = \underline{g}(t) \qquad (2)$$

where $\underline{a}_1$ and $\underline{a}_2$ are two vectors of constants and $\underline{g}(t)$ is a user-defined vector of functions of t.

The initial condition for Equation (1) is:

$$\underline{u} = \underline{u}_0(x) \qquad (3)$$

where $\underline{u}_0(x)$ is a user-defined vector of functions of x.

The generic method of solution of Equations (1) to (3) is the numerical method of lines. The specifics of the implementation include:

- The derivatives with respect to x are replaced with algebraic approximations by collocation on cubic hermite basis functions.
- The integration of the resulting initial-value ordinary differential equations (ODEs) in t is by the IMSL routine DGEAR modified for implicit ODEs of the form $\underline{A}\underline{dy}/dt = \underline{f}(\underline{y},t)$.

Initial experience with DPDES indicates the following desirable features and limitations:

Features

- No inherent limit on the number of simultaneous PDEs (the limit is imposed by the memory of the host computer and the computer run times).
- Coding of a PDE problem is straightforward.
- DPDES is available at most mainframe and minicomputer centers because of the wide availability of IMSL.

Limitations

- The PDEs are limited to one spatial dimension.
- The highest order derivative in x permitted [in Equation (1)] is second order.
- The boundary conditions must be linear and in the form of Equation (2).
- The initial and boundary conditions must be compatible (this requirement is subsequently explained in terms of an example).
- The user must provide the derivative of $\underline{g}(t)$ with respect to t in Equation (2).
- The user must provide $\underline{u}_x(x,0)$ even though this is generally not part of the problem system specification. However, $\underline{u}_x(x,0)$ can be selected in most cases to insure compatibility between the initial and boundary conditions.
- Only PDE problems with relatively smooth solutions can be accommodated. Thus PDES is intended primarily for parabolic problems and mildly hyperbolic PDEs. It cannot, for example, handle hyperbolic PDE solutions which exhibit steep, moving fronts and discontinuities.
- Only evolutionary PDEs can be accommodated; i.e., PDEs with an initial-value independent variable, t in the case of Equations (1) to (3). Thus DPDES cannot handle elliptic problems (the second reason for this conclusion is that elliptic problems are usually two dimensional). Also, simultaneous PDEs must be explicit in the initial-value independent variable, e.g., coupling between the derivatives in $\underline{u}_t$ is not permitted.
- Initial use of DPDES appears to indicate it is relatively inefficient in computer time when compared with other method-of-lines codes for the particular test problems used. However, this situation could change depending on the stiffness of the resulting ODEs for a particular problem since DPDES does have a state-of-the-art initial-value integrator (a variant of DEGEAR).

*IMSL is a collection of quality FORTRAN subroutines for a broad spectrum of mathematical and statistical calculations that is available commercially at modest cost; information is available from IMSL Inc., Sixth Floor - NBC Bldg, 7500 Bellaire Blvd, Houston, TX 77036-5085.

A Model PDE Problem

The development of codes for PDEs has progressed rapidly in recent years so that now several transportable codes are available. The next logical step in this development therefore appears to be the comparative evaluation of the codes. In order to move toward this goal, standard test problems should be used in comparative studies. A test problem is herein proposed and then used to illustrate a few special requirements of subroutine DPDES.

The one-dimensional hyperbolic-parabolic (convective-diffusion) PDE:

$$u_t = u_{xx} - (Pe)u_x - c*u^p \qquad (4)$$

contains a parameter, Pe, which can be used to change the character of the equation. For small Pe, Equation (4) is strongly parabolic while it is strongly hyperbolic for large Pe so that the difficulty of computing a solution to Equation (4) increases with increasing Pe; in fact, Equations (1) to (3) are impossible to integrate by any numerical method for any arbitrarily large, but finite, Pe.

The auxiliary conditions proposed for Equation (4) are:

$$1 = u(0,t) - (1/Pe)u_x(0,t),$$

$$u_x(1,t) = 0 \qquad (5)\ (6)$$

$$u(x,0) = 0 \qquad (7)$$

Equations (4) to (7) are the proposed standard test problem with the following special cases:

1) p = 1 (linear), c = 1, Pe = 10 (strongly parabolic)
2) p = 1 (linear), c = 0, Pe = 10 (strongly parabolic)
3) p = 1 (linear), c = 0, Pe = 100 (moderately parabolic and hyperbolic)
4) p = 2 (nonlinear), c = 1, Pe = 10 (strongly parabolic).

Finally, the application of subroutine DPDES to Equations (4) to (7) requires compatibility of the initial and boundary conditions and the specification of $u_x(0,t)$; the latter is not part of the stated problem.

Both requirements can be met by taking $u_x(0,0) = -Pe$, $u_x(x > 0,0) = 0$; these conditions follow from Equations (5) and (7). A solution to Equations (4) to (7) was then produced by subroutine DPDES. A commented FORTRAN program illustrating the details of calling DPDES is available from the author on request.

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GPA COMPUTER PROGRAMS

The Gas Processors Association, 1812 First Place, Tulsa, OK 74103, (918) 582-5112, has available in FORTRAN source code on magnetic tape with documentation the following commercial-grade software (most at special prices for universities):

Program	Brief Description	Special Price
GPA*SIM	Interactive "super flash" program for light gas-acid gas-hydrocarbon-water systems, based on the use of a modified Soave-Redlich-Kwong equation of state.	$500
GPA/OSU Soar Gas Equilibria	Equilibrium calculations for acid gas-ethanolamine treating solutions	$500
GPA Cryogenic Solubility	Solubility of CO_2 and hydrocarbons in cryogenic LNG and NGL with S-L-V phases.	$100
GPA Liquid Properties '80	Thermodynamic properties of liquid mixtures of light gases and paraffin hydrocarbons	$100
GPA TRAPP	Viscosity, thermal conductivity, and density of gas and liquid mixtures of natural gas and other hydrocarbon mixtures over wide ranges of T and P	$50
GPA/NASA Chemical Equilibria	Chemical equilibria	$100
K-Value Computer Program	Curve-fitted coefficients and computation method for K-values of 12 major hydrocarbons at various convergence pressures	$100

Further information on these programs can be obtained from the GPA who also market the EQUI-Phase program that uses the Peng-Robinson equation of state.

SYSOPT - OPTIMIZATION PROGRAM FOR APPLE II

by M. Rijckaert

SYSOPT is a software package designed for solving the following problem on an Apple II+ microcomputer:

Find the vector variable which minimizes the function

$$i(x)$$

while satisfying constraints

$$q_i(x) = 0 \qquad i = 1,.....,m$$

$$h_i(x) = 0 \qquad i = 1,.....,p \ .$$

In the absence of the latter conditions, the problem is termed unconstrained. Otherwise, it is called a constrained problem.

Because of the presence of default options and standard procedures, NO prior knowledge about the computational techniques is required. On the other hand, an experienced user can take full advantage of the modular structure of SYSOPT by tailoring the method to his particular needs.

SYSOPT offers the following optimization algorithms:

* **unconstrained optimization:**
  a. one-dimensional search
     - Fibonacci
     - Davies, Swann & Campey
     - Fletcher
  b. n-dimensional optimization
     - Rosenbrock & Palmer
     - Powell
     - Fletcher & Reeves
     - Davidon, Fletcher & Powell (DFP)
     - Complementary DFP algorithm (BFGS)

* **constrained optimization**
     - Penalty functions
     - Augmented Lagrangian Method

General information on SYSOPT.
The problem formulation consists of the definition of the objective function and of the equality and inequality constraints. Eventually the gradients of the objective function should also be stated. Each part of the problem formulation has to be defined in a subroutine according to the rules outlined in the manual. The objective function f(X) can be given by an analytical expression or by a recursive relation. It is also possible to introduce the function values directly.

The user can determine the appropriate output slot by answering the related question, which will appear on the screen in due time. For a problem with more than 10 variables, it is advisable to direct the intermediate results to the printer because of space limitation on a screen. Gradient values will only be communicated if the output is directed to a printer.

SYSOPT will propose a standard procedure which can be accepted or rejected. If the proposed procedure is rejected, the user will be able to put together another procedure selected through a series of menus. When all selections are made, the user can have the chosen procedure registered as the future standard.

For an algorithm based on derivative values, one can choose to use either numerically or analytically derived gradients. If the appropriate analytical expressions are not given, a numerical estimate is made based upon the central difference method. The program provides the possibility to check the correctness of the analytical derivatives at the start of the execution of the program.

For each algorithm, default options are provided for the stopping criterion. These options can eventually be changed by the user. The same is true for all heuristic parameters that need to be introduced.

For Fletcher-Reeves, DFP, and BFGS, the possibility exists of restarting the algorithm after each n+1 iteration.

Constrained Optimization
The only techniques made available here are methods which make extensive use of unconstrained minimization. SYSOPT offers the penalty function technique and the augmented Lagrangian method. The penalty function method (SUMT) handles inequality constraints through an interior approach and equality constraints through an exterior approach. The algorithm has a Phase-I procedure to generate a point which is interior for the inequality constraints.

The augmented Lagrangian method uses exterior penalty terms. Initial values for the Lagrange multipliers may be user supplied or estimated by a first-order method. Two alternatives are provided to update the multipliers.

The constrained optimization algorithms are allowed to use only those unconstrained procedures which use gradient information. No limitation is placed on the choice of the line search.

Areas of Application
- minimizing production cost functions
- minimizing energy cost functions
- optimal design
- solution of systems of nonlinear equations

Manual
A typewritten manual is provided, together with a manual written as a file for the Apple Writer and residing on the same disk as the SYSOPT program.

SYSOPT is available to educational institutions at a price of US $200.

Please contact:

Professor M. Rijckaert
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de Croylaan 2
B-3030 Heverlee
Leuven, Belgium

PROGRAMS FOR HAND-HELD PROGRAMMABLE CALCULATORS

The CACHE booklet entitled **"Hand-Held Programmable Calculators: A Review of Available Programs for Chemical Engineering Education,"** by Professor F. William Kroesser of West Virginia College of Graduate Studies, is still available. In this 26-page booklet, approximately 100 programs are listed under the following subjects:

THERMODYNAMICS
- Thermodynamic Properties
- Equations of State
- Equilibria

TRANSPORT PHENOMENA
- Viscosity
- Bernoulli Equation
- Pipe Flow
- Open Channel and Wier Flow
- Conduction
- Convection
- Radiation
- Diffusivity

UNIT OPERATIONS
- Distillation
- Absorption
- Humidification and Cooling

PROCESS DESIGN AND CONTROL
- Control Valve Size
- Fluidized Beds
- Compressors

Given for each program listed are 1) a description, including restrictions, 2) a literature reference to the program listing, and 3) a summary of input and output data. Sources of the programs are the HP67/97 Users' Libraries, the TI58/59 Program Exchange Club and specialty booklets, and articles in Chemical Engineering, Chemical Engineering Progress, Hydrocarbon Processing, and the Oil and Gas Journal.

An order blank for Professor Kroesser's booklet is included at the end of this issue of CACHE News.

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The following companies have contributed financial support to specific CACHE activities during 1982-84:

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CACHE COMPUTER PROGRAMS FOR CHEMICAL ENGINEERING STILL AVAILABLE

In 1972, CACHE published seven volumes of "Computer Programs for Chemical Engineering." The volumes covered the following areas: Stoichiometry, Kinetics, Control, Transport, Thermodynamics, Design, and Stagewise Computations. Each volume contains descriptions and listings of from 11 to 24 tested FORTRAN programs prepared by eminent chemical engineering educators. The programs have proven useful for homework problems, classroom demonstrations, design laboratories, and process simulation. The seven volumes are still available individually at prices ranging from $12.95 to $14.95, and as a complete set at $89.95. Complete information on the volumes is available from the current publisher:

Sterling Swift Publishing Company
P. O. Box 188
Manchaca, TX 78652

AICHEMI MODULAR INSTRUCTION SERIES AVAILABLE

AIChE is publishing one volume per year of each of the AICHEMI Modular Instruction Series listed below. The series were prepared by CACHE under the direction of Professor Ernest J. Henley of the University of Houston and William A. Heenan of Texas A and I University.

Series

A. Process Control: T. F. Edgar, Editor
B. Stagewise and Mass Transfer Operations: E. J. Henley, Editor
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The modules were designed to be used for outside study, special projects, entire university courses, review courses, correspondence courses, continuing education courses, or to provide new and timely material that can supplement other courses. A tentative outline listing titles and authors of all modules appears in the volume distributed to all chemical engineering departments. The volumes are available from:

Publications Department, AIChE
345 East 47 Street
New York, NY 10017

by single volume or by subscription.

CACHE REAL-TIME COMPUTING MONOGRAPHS BEING CLOSED OUT

MONOGRAPHS BEING CLOSED OUT AT $15/set + postage and handling

In 1977, the CACHE Real-Time Computing Task Force, under the direction of Professor Duncan Mellichamp prepared eight monographs on the following topics in Real-Time Computing.

MONOGRAPH I AN INTRODUCTION TO REAL-TIME COMPUTING

0. Digital Computing and Real-Time Computing Digital Computing (Mellichamp)
1. The Structure of Real-Time Systems (Mellichamp)
2. An Overview of Real-Time Programming (Mellichamp)

MONOGRAPH II PROCESSING, MEASUREMENTS, AND SIGNAL PROCESSING

3. Processes and Representative Applications (Edgar)
4. Measurements, Transmission, and Signal Processing (Wright)

MONOGRAPH III INTRODUCTION TO DIGITAL ARITHMETIC AND HARDWARE

5. Representation of Information in a Digital Computer (Fisher and Seborg)
6a. Digital (Binary) Logic and Hardware (Engelberg and Howard)

MONOGRAPH IV REAL-TIME DIGITAL SYSTEMS ARCHITECTURE

6b. Digital Computer Architecture (Engelberg and Howard)
7. Peripheral Devices and Data Communications (Rudd)
8. Digital Computer/Process Interfacing (Hughes)

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9. Assembly Language Programming (Fisher)
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16. System Operations Management and Program Documentation (McCarthy and Weaver)

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A. Process Analysis and Description (Edgar)
B. Digital Computer Control and Signal Processing Algorithms (Edgar and Wright)

These monographs are intended for use in lab courses, in self-study, and by real-time users at all levels because they contain many detailed examples. The monographs have been in heavy demand, particularly due to the trend towards use of real-time computing in the undergraduate laboratory. The monographs are being used as texts in a numer of universities and are available as single volumes at $3.75. Complete sets are now being closed out at $15.00, plus postage and handling from

Professor Brice Carnahan
CACHE Publications Committee
Chemical Engineering Department
Dow Bldg, North Campus
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Ann Arbor, MI 48109

An order form appears at the end of this Newsletter.

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