CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 19

September 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 D. M. Himmelblau with contributions from a number of CACHE members and representatives.

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MESSAGE FROM THE PRESIDENT
by R. S. H. Mah
Northwestern University

Fifteen years ago a group of young educators met at Michigan University to consider the problem of introducing computer aids to chemical engineering education. This meeting resulted in the formation of the CACHE (Computer Aids for Chemical Engineering Education) Committee, the forerunner of CACHE Corporation. Since that time CACHE has

1. developed standards for computer programs;
2. compiled and published 7 volumes of computer programs for the core chemical engineering courses written by about 100 chemical engineering professors;
3. prepared a complete set of modular instructional materials for the core chemical engineering courses;
4. published a series of monographs on real time computing;
5. introduced the use of FLOWTRAN, a Monsanto design program, to more than 50 chemical engineering departments and thousands of students;
6. co-sponsored the development of MicroCACHE, a lesson authoring and delivery software system for IBM PC and Apple computers; and
7. organized an international conference on computer aided process design.

To our friends, the generation of chemical engineers who grew up on FLOWTRAN, so to speak, CACHE seems like a part of the permanent landscape. It is hard to realize that the scenery was once quite different.

To mention just one of the dimensions of change, when CACHE was first formed in 1969, practically all computing was done on mainframe computers. Today we have micros, minis, mainframes, supercomputers, networking, graphics, laboratory applications, and so on. The computing environment is far more complex and challenging. But there are also many more opportunities for new initiatives and new directions. To respond to these challenges CACHE has regrouped its task forces and streamlined its efforts.

The project activities of CACHE have always been carried out by its task forces, organized to accomplish specific objectives. In the past year or so 7 of these task forces have completed their missions. In their places we have constituted 3 new ad hoc committees. Ad hoc committees are the embryos of task forces. They are formed to develop the project goals and plans before the task forces are created. In this vigorous stage of growth they need new personnel and new ideas.

You can help. If you are interested in the activities of a particular CACHE project, please feel free to approach the task force or committee chairman and ask to be invited to the task force meetings where the real action goes on. The only qualifications required of task force membership are interest and participation. If you have an idea which may or may not fit in with an existing CACHE project, please contact any CACHE trustee or officer. We would like to hear from you.

Our track record shows that CACHE has been extremely effective in translating ideas into reality.

In this and past issues of CACHE newsletters you will find the descriptions and progress reports of various task forces and ad hoc committees.

We hope you will join us.

CHEMICAL PROCESS CONTROL CONFERENCE

The third Chemical Process Control Conference (CPC-III) will be held in Pacific Grove, California, during the week starting January 12, 1986. CACHE will sponsor CPC-III. Two predecessor conferences have been held, one in Pacific Grove in 1976 and the other at Sea Island in 1981.

To permit adequate discussion, both scheduled and unscheduled, the number of attendees will be limited to approximately 125. Formal sessions will be held in the morning and evening. The general topics to be included in the conference are listed below.

This third conference will focus on advances that have taken place in the process control field over the last 5 years. In particular, developments in the areas of control system robustness, process operability, adaptive control, and model predictive control will be highlighted. Actual industrial applications of advanced control will be discussed. Finally, one session will take a speculative look at the future of process control, in particular the potential impact of artificial intelligence and parallel computing and new ideas for process control education.

MONDAY
A.M. Control in the Presence of Constraints. Deadtime and Uncertainty-Theoretical Advances
P.M. Industrial View of Advanced Process Control
TUESDAY
A.M. Adaptive Control
P.M. Identification and On-Line Optimization
WEDNESDAY
A.M. Process Operability
P.M. Process Control Software: Needs and Capabilities
THURSDAY
A.M. Reactor Control
P.M. Speculations on the Future of Process Automation, Operation, Control, and Education
FRIDAY
A.M. Summary
For further information write CPC-III, CACHE Corporation, P. O. Box 7339, Austin, TX 78713-7339.

MICROCACHE PROJECT
by B. Carnahan
University of Michigan

Finally! The MicroCACHE CAI software (see the April 1984 CACHE Newsletter) is about to be released to Chemical Engineering departments. The initial “Introduction to MicroCACHE 1.0” package will consist of:

a. module preparation software (on diskette)
b. module presentation software (on diskette)
c. data retrieval software (on diskette)
d. two sample modules (on diskette)
e. documentation (five manuals)

All materials will be for operation on either an IBM PC or PC-XT (and probably the PC-AT) equipped as follows:

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. monochrome (mono or color)
5. 8087 coprocessor chip (optional)
6. matrix printer (optional)
7. PC-DOS 2.0 or 2.1

The software will probably run on many PC “compatibles” operating under MS-DOS 2.0 as well, but we can’t guarantee that. The color/graphics adapter board is essential (i.e., MicroCACHE won’t run successfully using the IBM monochrome monitor board, since that board cannot handle bitmapted graphics on the associated alphanumeric monitor).

We suggest the use of the coprocessor since our 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.

I (and one of my students, Chris Jaeger) described the MicroCACHE software in Session 41 on Microcomputers in Education at the AIChE meeting in Anaheim in May. Write me at the following address for a reprint if you are interested in getting an overview of MicroCACHE System capabilities. (We have made some changes in the software since then, but MicroCACHE performs essentially as described in the article.)

Chemical Engineering Department
Dow Building, North Campus
University of Michigan
Ann Arbor, MI 48109

CACHE REPRESENTATIVES’ RECEPTION
SAN FRANCISCO AIChE MEETING

The annual reception and program for CACHE representatives and their guests will be held from 5:00 to 7:00 p.m. on Wednesday, November 28, in the Cypress Room of the Hilton Hotel at the San Francisco meeting. This session will feature a poster session highlighting the current and future activities of CACHE. Newly-elected CACHE President, Richard S. H. Mah, will briefly discuss the current status of CACHE activities and introduce Task Force chairmen.

Special efforts will be made to interest and involve more of the CACHE representatives in various CACHE activities. The poster session will allow representatives to obtain information and discuss their individual interests in an informal manner. Examination copies of available CACHE publications will be available. All of these activities will be accompanied by moderate amounts of wine and cheese.

More details on the CACHE Representatives’ Session will be sent to representatives and department chairmen prior to the San Francisco meeting.

AUTHORING SYSTEMS FOR COMPUTER-BASED INSTRUCTION
by M. B. Cutlip
University of Connecticut

The coming of the personal computer has greatly increased the ability to deliver computer-based instructional materials quite inexpensively. While the first educational systems required large mainframes with direct or telephone communications, the largest generation relies on the personal computer for authoring and delivery of instructional materials. A wide variety of software now exists for the creation of materials. A listing of current authoring systems is given below. A wide range of formats currently exists for the actual materials. In general, the easiest to use authoring systems are the most limiting. A variety of hardware is required for the current listing, but the trend is definitely toward compatibility with the IBM PC. In the future, new languages such as C will provide transportability to a wide variety of delivery machines.

The novice author is well advised to consider that the time to create quality educational materials is still rather severe. While the hardware and software costs have been falling in recent years, the time to produce viable materials in this exciting new medium remains very considerable.

Every effort has been made to make this listing as complete as possible; however, neither the author or CACHE Corporation are responsible for any errors or omissions. The author welcomes any additions or corrections and will maintain an updated listing which will be available upon request.
MicroTCIT
Hazeline Corporation
Training Systems Center
7680 Old Springhouse Road
McLean, VA 22102
(703) 827-2300

MICROINSTRUCTOR
Mosby Systems
11230 Westline Industrial Drive
St. Louis, MO 63146
(314) 325-4177, Ext. 750

THE EDUCATOR
Spectrum Training Corporation
18 Brown Street
Salem, MA 01970
(617) 741-1511

VAX PRODUCER
Digital Equipment Corporation
Educational Services
30 North Avenue
Burlington, MA 01803
(617) 276-1454

C. A. S. IVIS
Digital Equipment Corporation
Education Computer Systems
2 Iron Way
Marlborough, MA 01752

DuoSoft MicroTUTOR
DuoSoft Corporation
1805 Woodfield Drive
Savoy, IL 61874
(217) 356-7524

PILOTplus
Online Products Corporation
20251 Century Boulevard
Germantown, MD 20874
(301) 428-3700

OMNISIM
Instructional Systems Group
302 Students' Union Building
University of Alberta
Edmonton, Alberta
Canada T6G 2H1
(403) 432-2611

CAN-8
Honeywell Information Systems Inc.
200 Smith Street, MS 433
Waltham, MA 02154
(617) 328-5111, Ext. 2712

R2-C
Regency Systems, Inc.
P.O. Box 3578
Champaign, IL 61821
(217) 398-8087

The PHOENIX System
Goal Systems International Inc.
5455 N. High Street
Columbus, OH 43214-1193

EnCORE
Computer Teaching Corporation
1713 S. Neil
Champaign, IL 61820
(217) 398-2207

PASS Authoring System (Apple)
MVA Authoring System (IBM PC)
Bell & Howell
Visual Communications
7100 N McCormick Road
Chicago, IL 60645
(312) 673-3300, Ext. 4674

PLATO Authoring System
Control Data Corporation
P.O. Box O - HQAO2I
Minneapolis, MN 55440
(800) 828-1109

WISE Authoring Software
Wiscat Systems
P.O. Box 539
Orem, UT 84057
(801) 224-6400

Ghostwriter Authoring System
Cavi V Authoring System
Cavi
26 Trumbull Street
New Haven, CT 06511

CACHE MICROCOMPUTER/
PERSONAL-COMPUTER NOTES

edited by P. R. Rony
Virginia Polytechnic Institute
& State University

Faculty members who wish to stay abreast of the computer literature may be interested in the biweekly publication, Computer Contents (Management Consultants, 2285 Carlson Drive, Northbrook, II. 60062). The tables of contents of 350 computer periodicals are reproduced. The cost is $95.00 per year (26 issues) for U.S., Canada, or Mexico.

Virtual Microsystems Inc. (Berkeley, CA) is selling for $1750 a conversion board that adds PC-DOS capability to DEC's Professional 350 and Micro-11 computers. The board, called PC-Bridge, contains an 8 MHz 8086, 256 Kbytes RAM, and fully emulates an IBM PC color graphics card. Programs can therefore be run that take advantage of the IBM PC bitmapped graphics memory. For further details, consult the 1.3-page announcement in Mini-Micro Systems, August 1984, pages 54, 58.

A general discussion [Mini-Micro Systems, July 1984, pages 97-99, 103-104] entitled, "Hardware Differences Can Make or Break the 50 IBM PC-Compatible Manufacturers," makes the point that the MS-DOS and PC-DOS memory architectures differ. A generalized memory map is provided. "A noticeable difference
between MS-DOS and PC-DOS is the BIOS, which IBM chose to divide into hardware and firmware.” Details are lacking in the article, but some insight into why many PC “clones” are incompatible is provided.

A user of electronic mail soon encounters the term, “gateway,” which is a connection between two or more computer networks. An interesting article on the subject, entitled “Gateways: Link Long-Haul and Local Networks,” can be found in Data Communications, July 1984, pages 111-122. In the same issue is an article, “Putting a Price on File Transfer” [pages 177-187], that compares the costs for five different schemes for linking personal computers to mainframes: (1) dedicated asynchronous modems, (2) protocol converter, (3) bisynchronous adapter, (4) coaxial interface, and (5) terminal conversion. The total reported costs for seven users is $60,750, $65,070, $76,650, $72,172, and $96,151. No wonder users are not making such links.

At Virginia Tech, we purchased a Data Lynx protocol converter ($1800); dedicated a Heath Z809 personal computer ($2300) to a personal-computer-to-mainframe link, paid monthly rental charges for a 9600-baud modem/data switch and dedicated line (about $50 per month) and thus created a facility that permitted students to upload FORTRAN programs on floppy disks to an IBM mainframe.

A discussion, “Shrinking VMS,” concerning how the Digital Equipment Corporation Virtual Memory System (VMS) operating system was shrunk to become the MicroVMS operating system on a MicroVAX, is given in the July 15, 1984 issue of Datamation, pages 95-100. The same issue contains an article on “Computer Conferencing” [pages 111-116]. Conferencing vendors include The Source, CompuServe, Infomedia Corporation, Tymshare, Cross Information Company, Advertel, The Electronic Information Exchange System, ITT Dialcom, and Participation Systems Inc. The Electronic Information Exchange System, available from the New Jersey Institute of Technology (Newark, N.J.), is a resource for exploring and developing computer conferencing.


Michael Andrews’s book, “Programming Microprocessor Interfaces for Control and Instrumentation” [Prentice-Hall, 1982], has two nice chapters on Data Acquisition (Chapter 9) and Process Control Digital Algorithms (Chapter 9). Useful 8089 microprocessor listings are provided: they can be adapted to other microprocessors.

The August 21, 1984 issue of PC features a series of articles on Robotics and Process Control. One of the cover stories, “A Computerized Notebook for Scientists” [pages 134-139], features a product called LABTECH NOTEBOOK that is made by Laboratory Technologies Corporation, 328 Broadway, Cambridge, MA 02139. Fred Putnam, a chemical engineer and president of the company, reported on this product for the first time at a CAST session at the spring 1984 Anaheim ALChE meeting. The $795 software package (significant discounts to chemical engineering educators) simplifies the acquisition of data by a hardware data acquisition board that is added to an IBM PC. What is interesting is the availability of a customized version of Lotus 1-2-3 that facilitates graphics and tabular comparisons. A graduate student, Mr. P. Kip Mercure, at Virginia Tech has the following comments about the software: “Can acquire up to 8000 samples/second. Good for long-term batch experiments, for example, those that last for hours. A nice feature is the chart recording that appears on the screen (however, it has some bugs such as axis mislabeling).” In the continuum between computer-based data acquisition and process control, LABTECH NOTEBOOK is primarily oriented toward data acquisition. Well integrated, easy to set up, and easy to use. Software has a niche: a reasonable first effort.”

PC World magazine publishes two special editions, Annual Hardware Review and Annual Software Review, that summarize commercial IBM PC hardware and software. The latest editions are 1984 and 1983-1984, respectively. Price, $4.50 each issue, available from PC World Communications, Inc., 555 De Haro Street, San Francisco, CA 94107.

Kermit is coming! In fact, they are already here. Two very interesting articles by Frank da Cruz and Bill Catchings, “Kermit: A File-Transfer Protocol for Universities - Part 1: Design Considerations and Specifications, and Part 2: States and Transitions, Heuristic Rules, and Examples,” which appear in the June and July 1984 issues of Byte [pages 255-278, 1143-145, and 400-403], describe a file-transfer protocol that was developed at Columbia University for downloading files from mainframes to microcomputers. The Kermit protocol has evolved into a comprehensive communication system for transferring data between numerous types of computers. For example, the editor could get an IBM PC Kermit and a Zenith Z89 Kermit to transfer files between the two indicated computers. For details, write to Kermit Distribution, Columbia University Center for Computing Activities, 7th Floor, Watson Laboratory, 612 West 115th Street, New York, NY 10025.

Hugh Kenner, writing in BUSS #88 (The Independent Newsletter of Heath Company Computers), the following Kermit that he has created: Z-DOS for the Z100, PC DS for the IBM and its clones; CP/M 80 for the Z100, and CP/M 2.2 for the H89 (hard sector only). He states: “Remember, you need a Kermit for each machine...there seems to be no IODOS Kermit yet.”

The June 1984 issue of Byte magazine features “Computers and Education—On Every Desk, in Lab and Field.” Among the featured articles is the thoughtful four-page article, “Languages for Students,” by Fred A. Masterson [pages 233-238].
The successor to Pascal is Modula-2, a language also developed by Niklaus Wirth. The August 1984 issue of *Byte* features Modula-2 and includes an article, "History and Goals of Modula-2," by the developer. Volume 9, Number 9 is a special issue of *Byte* that is a "Guide to the IBM Personal Computer," including the IBM PC, IBM PC XT, IBM PC Portable, IBM XT/370, IBM 3270, and IBM S9000.

An article, "The Compatibles Line Up," by Robert Luhn in the April 1984 issue of *PC World* [pages 102-125] provides a table that compares 45 desktop or portable/briefcase compatibles in terms of list price, processor, 8087 socket, RAM (min. and max.), ports, PC expansion slots, disk drives (size, storage, density/ade), power supply, display (type, resolution, colors, format), keyboard (IBM layout, fully definable, full IBM character set, function keys), operating system, software included, and hardware included. Only the most recent IBM PC clones are covered.

The August 1984 issue of *PC World* describes Perfect Software's Perfect Link communications program, which includes a helpful utility for converting data between CP/M and PC-DOS. See pages 242-244. The September issue of the same magazine has an interesting article, "Intelligent Communications," that compares five all-purpose smart terminal communications packages for the PC: Telcom, Relay, Omnitemr 2, Blast, and Crosstalk XVI [pages 166-175]. Also appearing in the September issue is a comparison of five new statistical packages: AbStat, Crisp, Microstat, SL-Micro, and Systat [pages 186-195].

The most effective and popular exhibit at the July National Computer Conference (NCC'84), in the editor's opinion, was the Apple Computer booth. Twenty or thirty different software packages for the Macintosh were featured, approximately ten new ones every two days. It was probably the only booth you could revisit and find something new. The new publication, *Macworld*, from those same folks who publish *PC World*, is very slick and certainly does a fine job of featuring the special graphics characteristics of the Macintosh. With 24 universities and colleges in the Apple consortium, many of you who read this may already have a Macintosh.

A fascinating publication is DTACK GROUNDED (The Journal of Simple 68000/16081 Systems), one of the few publications that I read immediately from front to back. In addition to discussing hardware developed by the parent company, Digital Acoustics, the editor of the publication discusses a variety of timely topics that are of interest to faculty members who wish to stay on top of the rapidly evolving personal computer market: the success (or lack of success) of UNIX, Macintosh, new IBM PCs, 32-bit workstations, 68000-based microcomputers, Kindly Uncle Jack (Tramiel), Intel 80286 products, and so forth. Issue #35 (September 1984) contains 26 pages of densely-typed material. Subscriptions are $15 for 10 issues in the U.S. and Canada. Make the check payable to DTACK GROUNDED and send it to 1415 E. McFadden, Sta. F., Santa Ana, CA 92705.

**COMMUNICATIONS AD HOC COMMITTEE**

by P. R. Rony
Virginia Polytechnic Institute & State University

While selected chemical engineering professionals already have access to a computer network—most likely within a company but perhaps even a national network such as ARPNET—there is currently no national chemical engineering network between educational, industrial, and government institutions that is analogous, for example, to CSNET, which is used by computer science and engineering professionals, or in COMPMAIL+, which is used by members of the IEEE Computer Society.

COMPMAIL+ provides a useful model that can be tested immediately by the chemical engineering community. Officers and staff of the Computer Society have been experimenting with electronic mail for almost two years (they started with Telenet but more recently moved to ITT Dialenum and its more cost-effective COMPMAIL+ service). They have found the following ITT Dialenum services to be particularly helpful:

a. Mail drop capability, in which a user can send messages by a local phone call to a central computer in Maryland, which routes the message to the "mailboxes" of other recipients.

b. Mailing list capability, in which a user can send his message to many recipients simultaneously. Electronic "carbon copy" capability also is provided.

c. Quick response: a completed message is immediately placed in the mailbox of a recipient.

d. Message storage: the ability to store both transmitted and received messages for later recall.

e. Message forwarding: the ability to "bounce" received messages electronically to other individuals.

f. Subgroup identification, in which a user can identify a group of recipients to receive messages, give the group a single identification name, and address the group with a simple 10 character code.

g. Archiving of communications: a single floppy disk can store all transmitted and received communications for future access.

Once chemical engineers become familiar with a national chemical engineering electronic mail service, it is quite likely that a number of special interest groups would use it for their rapid communications needs. Typical groups would include, for example,

- research engineers working in the area of catalysis
- chemical engineering department heads and chairmen
- organizers and/or participants of a conference
- chemical engineering laboratory instructors
- AIChE student chapter presidents
- CAST Division officers
- speakers at a specific AIChE meeting session
- the editor and manuscript authors of an AIChE journal
- candidates for department chairman at a given university
- CACHE board of trustees

Such groups would form naturally as the need for electronic mail arises. Bulletin boards of broad interest may also develop. The issue is not whether such activities will occur, but when.

Most of us do not have much experience with a national electronic communication (electronic mail) service. We do not know the features of alternative communication networks or their cost. It is not clear what would be the best choice for the chemical engineering community, both in the short term and the long term.

The objective of the CACHE Communications Ad Hoc Committee is to gather information on existing professional networks, to perform limited experiments and tests on selected networks, and to make recommendations to CACHE concerning a strategy for implementing a chemical engineering electronic mail service (CHEEMS). A report would be issued that documents concrete examples of how to use electronic mail; identifies potential chemical engineering applications (preferably educational applications); and lists typical costs. The document and the results of the experiments would be reported in the CACHE newsletter, the CAST newsletter, and perhaps even in CEP. Such information possibly could be used as a basis for future CACHE proposals to industry and government.

Though there is vigorous activity in the electronic mail area, it is still in a state of flux, so time is available—even one year—to do a proper study of opportunities and organizations.

PROPOSED ACTION PLAN

A preliminary action plan is presented here for the comments and suggestions of readers of CACHE News:

1. Select a group of five to seven individuals (at scattered geographical locations) who would be willing to (a) participate in a test of several electronic communications network services, or alternative approaches to networking, (b) collect information, and (c) write a report. Candidate electronic mail services include COMPMAIL+ (ITT Dialcom and IEEE Computer Society), BITNET, the University of Michigan network, a network that is based upon our own hardware, and perhaps other networks. CSNET and ARPANET appear to be too expensive for widespread chemical engineering use.

2. We would like to identify several colleagues from academia who would be interested in participating in our electronic mail experiments. We propose to use your activities as the basis for our experiments. Inquiries should come in the form of brief proposals that provide (a) the reason why rapid communication is needed by your interest group, (b) the general subject matter of your interest group, (c) the names of the individuals in your group, and (d) the availability of departmental financial support so that we could maximize the use of CACHE funds. CACHE is considering a $1000 expenditure to fund a limited experiment involving such a group. Several CACHE trustees, including Rudy Motard (Washington University, St. Louis), John Hale (DuPont), and Peter Rony (on sabbatical leave at the University of Delaware), will oversee the experiment and perhaps participate in the writing of the report. Please mail your proposal to Dr. Peter R. Rony, Department of Chemical Engineering, University of Delaware, Newark, DE 19716.

3. Select several electronic mail or communications services, enroll the test group, and initiate the experiments for a short period of time, for example, several months. Write and disseminate a report that summarizes the results of the experiments.

PROPOSED FUTURE ACTIVITIES:

Identify a preferred electronic mail/communications service and plan a more ambitious experiment that involves users from many different chemical engineering work sites. Each work site would be responsible for financing. No further CACHE funds would be used.

TASK FORCE FOR THE DEVELOPMENT OF PROCESS DESIGN CASE STUDIES

by Ignacio Grossmann
Carnegie-Mellon University

The CACHE Task Force on Process Design Case Studies, under the direction of Professor Manfred Morari, has completed several activities.

The case study, “Separation System for Recovery of Ethylene and Light Products From a Naphtha-Pyrolisis Gas System,” has been completed by Professor Ignacio Grossmann and should be available for distribution in October, 1984. The report includes preliminary design calculations 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. To order copies of this case study, please contact.
Two other case studies are under preparation. One is on the problem, "Design of Ammonia Synthesis Plant," that was supplied by Mr. Philip Ruziska from Exxon Chemicals, and which is being prepared by Professor Ignacio Grossmann. The other case study is on the problem, "Production of Acetaldehyde by Dehydrogenation of Ethanol," supplied by Mr. David Witherrill from Union Carbide. Professor Lorenz Biegler is currently evaluating reports that have been submitted on this problem by Professor Bruce Finlayson, Professor Rakesh Govind, and Professor Richard Hughes. The final reports for these case studies should be completed early next year.

Problem statements are currently available on "Alcohol Isolation System" and "Solvent Recovery System," supplied by Dr. Jeffrey Sirola from Eastman Kodak. Statements for new case studies will be available by December 1984. For information on these design problems, or for anybody interested in submitting a report, please contact:

Professor Manfred Morari
Department of Chemical Engineering
California Institute of Technology
Pasadena, CA 91125

or

Professor Ignacio Grossmann
Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213

For potential contributors, it should be pointed out that the CACIIE Case Studies are to be tutorial with both the instructor and the student in mind. The problems should usually be loosely defined; a flowsheet will often not be specified. The goal is not necessarily to present one "optimal" solution, but possibly several alternatives with different attractive features. One section of the report should show in detail the steps, starting from the problem statement, how alternate solutions were generated and discarded based on preliminary short-cut calculations and qualitative considerations, and how the number of alternatives is decreased by the designer as he progresses toward a final solution. The report should also demonstrate, if possible, the application of process synthesis and optimization techniques, as well as the use of process simulators.

FOCAP PROCEEDINGS


The weeklong meeting, featuring papers by leading academic and industrial researchers in the computer-aided design field, was sponsored jointly by the CAST Division of the AICHE and CACIIE, with support from the National Science Foundation and nine corporations and corporate foundations including: Chiyoda Engineers & Construction Co., Exxon Research & Development Co., The Halcot SD Group, Monsanto Co., Olin Chemicals Corp., Process Simulation International, Shell Companies Foundation, Tennessee Eastman Co., and Weyerhaeuser Co.

Professor Arthur Westerberg (Carnegie-Mellon University) and Dr. Henry H. Chien (Monsanto Co.) were the meeting cochairmen and served as editors of the Proceedings.

The Proceedings (a hardbound book of more than 1000 pages) contains all 22 papers presented during the meeting, plus summaries of the discussions held during each session. The titles of the major sessions were:

1. Keynote (Expert Systems)
2. Overview and Outlook for Process Systems Engineering
3. Progress in Data Base Development
4. Computational Algorithms
5. Physical Properties for Design
6. Nonsequential Modular Flowsheeting
7. Design and Scheduling of Batch Chemical Plants
8. Complex Single Unit Design (columns, reactors)
9. Operability in Design
10. Contributed Papers (various topics, e.g., scheduling, property prediction, nonlinear equation algorithms)

To order the:

Proceedings of
the Second International Conference on
FOUNDATIONS OF
COMPUTER-AIDED
PROCESS DESIGN

Arthur W. Westerberg, Editor
Carnegie-Mellon University
Henry H. Chien, Editor
Monsanto Company
CACHE Corporation, 1984

write:

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

The postpaid charge is $37.50 (please include payment or purchase order). See the FOCAP PROCEEDINGS form at the end of this newsletter.

SOFTWARE FOR MATRIX BANDWIDTH
REDUCTION

by W. E. Schiesser
Lehigh University

The solution of systems of linear algebraic equations is a fundamental calculation in chemical engineering, and
accounts for a substantial part of the computation done by chemical engineers. For example, most nonlinear problems are solved by the iterative solution of a system of related linear equations, typically by Newton's method and its variants which require the iterative solution of systems of linear algebraic equations until convergence to the solution of the nonlinear problem is achieved.

Consequently, improvements in numerical algorithms for linear algebraic equations are of practical interest. While such algorithms have been studied extensively since from at least the time of Gauss, and possibly earlier, algorithm development and improvement for linear algebraic equations remains a very active area of research, primarily because the size of the problems continues to grow and exceeds the practical capabilities of present-day computers, e.g., systems of 100,000 linear algebraic equations are not unusual in oil reservoir simulations.

The well-established direct methods, such as Gauss row reduction or the equivalent LU decomposition, require \( n^3 \) operations where \( n \) is the number of equations. Thus, as \( n \) increases, the number of operations increases very rapidly. For example, if \( n = 10,000 \), \( n^3 = 10^{12} \), and if the calculations are performed on a 100 megaflop supercomputer (10^8 floating point operations/sec), the computational time for this relatively modest problem is \( 10^{12}/10^8 = 10^4 \) seconds or approximately 2.5 hours.

The question then naturally arises of what can be done to cut down the computer time. The answer, generally, is to try to take advantage of any structure the algebraic equations might have; in practically all physical problems, such structure does exist and can be exploited effectively. For example, if the linear algebraic equations come from finite difference approximations of partial differential equations (PDEs) that model an oil reservoir, the algebraic equations will be block banded. Thus, the trick in solving the algebraic equations efficiently is to process the blocks iteratively, and take advantage of the bandedness of each block. This, however, leads to computer codes that are rather specific to the problem, and the associated equation structure. Ideally, general-purpose methods for exploiting equation structure should be used which substantially improve the efficiency of codes developed for chemical engineering calculations.

A general approach to increasing the computational efficiency of the solution of large sets of linear algebraic equations is to try to reduce the bandwidth of the coefficient matrix. If the bandwidth is \( m \), and the system of equations is of order \( n \) (the number of equations), the operations count for direct (Gaussian-type) methods is \( m^2 / 2n \) [1]. Thus, if \( m = 1000 \) and \( n = 10,000 \), the number of operations is \( (10^3)^2 / 2(10^4) = 10^{10} \) and the preceding estimated computer run time is reduced by a factor of 1/100 to 100 seconds. Clearly, the value of \( m \) is critical in achieving significant computational efficiency.

A second consideration, however, is how the bandwidth reduction is actually achieved. If \( n = 10,000 \), manual reordering of the equations is clearly impractical. Recently, algorithms have been proposed for reordering [2], [3], [4], and these algorithms have been implemented in computer codes that are routinely used in finite element analysis. However, very little use has been made of these techniques by chemical engineers.

Also, the existing bandwidth reduction algorithms and their associated computer codes are relatively complex. Collins [5] has reported an algorithm which is simpler than the earlier algorithms and appears to be about as effective.

An example of the application of Collins' algorithm to a 9 x 9 linear algebraic system is illustrated in Figure 1, where two coefficient maps are presented: (a) is the original algebraic system and (b) is the bandwidth-reduced system. In each case, the indices of the unknowns are tabulated across the top and the indices of the equations down the left side. For example, in the case of the first row of (a), equation (1) depends on unknowns 1, 2, 8, and 9. In the bandwidth-reduced matrix, the original equation (1) is now equation (4), but it still depends on unknowns 1, 2, 8, and 9. Note, however, that in (a) the matrix is full while in the case of (b), the matrix is banded with triangles of zeros in the upper right and lower left corners. The bandwidth reduction achieved with Collins' method is not particularly impressive in this case because the problem is small (9 x 9), however, the way in which the reduction occurs is illustrated, and we have found that larger problems which originally have nearly full coefficient matrices are substantially reduced in bandwidth (note that the matrix can appear to be sparse, but just a few "outliers" in the top right and bottom left corners will effectively give it a wide bandwidth).

Collins' algorithm has been implemented in a transportable prototype FORTRAN code that is available to educators for a nominal preparation charge by writing to the author. The code is provided on nine-track tape, and includes a user's manual; also, the tape contains a 100 x 100 application resulting from the approximation of the nine PDEs which model a four pass shell and tube heat exchanger. In this application, substantial bandwidth reduction does occur; the performance of Collins' method can also be compared with manual reordering of the algebraic equations to achieve bandwidth reduction.

The prototype code has not been applied to large problems, e.g., \( n = 1000 \) or larger; rather, it is intended to demonstrate some basic concepts in bandwidth reduction. Also, a comparison of Collins' method with the earlier algorithms [2], [3], [4] has not been performed.

REFERENCES

[1] Rice, J. R., Numerical Methods, Software and


1 2 3 4 5 6 7 8 9
1 0 0 0 0 0 0 0 1 1
2 0 0 0 0 0 0 0 2 2
3 0 0 0 0 0 0 0 3 3
4 0 0 0 0 0 0 0 4 4
5 0 0 0 0 0 0 0 5 5
6 0 0 0 0 0 0 0 6 6
7 0 0 0 0 0 0 0 7 7
8 0 0 0 0 0 0 0 8 8
9 0 0 0 0 0 0 0 9 9

(a)

1 2 3 4 5 6 7 8 9
1 X X X X X X X 1 X
2 X X X X X X X 2 X
3 0 0 0 0 0 0 0 3 X
4 0 0 0 0 0 0 0 4 X
5 0 0 0 0 0 0 0 5 X
6 0 0 0 0 0 0 0 6 X
7 0 0 0 0 0 0 0 7 X
8 0 0 0 0 0 0 0 8 X
9 0 0 0 0 0 0 0 9 X

(b)

Figure 1. (a) Original matrix; (b) Final matrix

STATUS OF FLOWTRAN LOAD MODULES
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-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 (68R2/08) 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:

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<th>Version</th>
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<th>FORTRAN Compiler</th>
</tr>
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<tbody>
<tr>
<td>a</td>
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<td>VS</td>
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<tr>
<td>b</td>
<td>OS1/MVS</td>
<td>IV Hx</td>
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<td>c</td>
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<td>VS</td>
</tr>
<tr>
<td>d</td>
<td>CMS</td>
<td>IV G1</td>
</tr>
</tbody>
</table>

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.

Conversions are also underway for the DEC 10, Honeywell, Sperry 90/80, Data General MV/8000, DEC VAX under UNIX, and Prime machines. Each FLOWTRAN tape contains either load and/or relocatable code, text programs 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 71 universities:

University of Akron
University of Arizona
Arizona State University
Brigham Young University
University of British Columbia
Bucknell University
University of California, San Diego
Case Western
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 Monsanta. 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.

LINDO-INTERACTIVE COMPUTER PACKAGE FOR LINEAR PROGRAMMING

by Ignacio Grossmann
Carnegie-Mellon University

LINDO (Linear INteractive and Discrete Optimizer) is an interactive computer program for solving linear programming and mixed-integer linear programming problems that involve 0-1 variables. The code has also provisions to handle quadratic programming problems through linear complementarity formulations.

The main advantage of LINDO is that it is very flexible, friendly, and easy to use. The program is a very useful tool for solving a variety of optimization problems, and it is particularly suitable for educational purposes.

The program accepts free form equation-type input as shown below:

@LINDO
.MAX 20A + 28B + 25C
>ST 2A + 3B + C = 100
> A > 25
> B < 40
> C < 30
>END

The answer to the problem is obtained simply as follows:

.GO
LP OPTIMUM FOUND AT STEP 4
OBJECTIVE FUNCTION VALUE
1) 1450.00000

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<tr>
<td>B</td>
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<tr>
<td>C</td>
<td>30.000000</td>
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REDUCED

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<td>4)</td>
<td>40.000000</td>
<td>0.000000</td>
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<tr>
<td>5)</td>
<td>0.000000</td>
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For large problems LINDO interfaces with MPS files (standard LP format) and with user-supplied FORTRAN subroutines. The package has over 40 commands, help features, capabilities for range (sensitivity) analysis and many display options.

Versions of LINDO are available for most mainframes; for instance, DEC-20, VAX, IBM, CDC/Cyber, Univac, Prime, HP3000, Data General. These versions can handle problems with up to 800 rows and 4000 variables. The price of these versions starts at $750 for educational users. There are also several versions for personal computers that are IBM compatible. Their price starts at $250.

Information about the LINDO computer package can be obtained from the author:

Professor Linus Schrage
Graduate School of Business
University of Chicago
1101 East 58 Street
Chicago, IL 60637
(312) 962-7449

Several books are also available for LINDO, and these include the following:

- User's Manual for LINDO, Linus Schrage
- Linear, Integer and Quadratic Programming with LINDO, Linus Schrage
- LINDO/PC System, Linus Schrage

These books can be obtained from:

The Scientific Press
450 University Avenue
Palo Alto, CA 94301
(415) 322-5221

CALENDAR OF EVENTS

DECEMBER 1984

4-6 1984 Real-Time Systems Symposium. Austin, Texas. Sponsor, IEEE-CS. Contact: Miroslav Malek, University of Texas at Austin, Computer Science Department, Austin, TX 78712. (512) 471-5704.

12-14 IEEE Decision and Control Conference. Las Vegas, Nevada. Sponsor, IEEE. Contact: Abraham Hashid, 23rd CTC School of Electrical Engineering, Georgia Institute of Technology, Atlanta, GA 30332. (404) 894-8930.


JANUARY 1985

2-4 Hawaii International Conference on System Sciences. Honolulu, Hawaii. Sponsors University of Hawaii and University of Southwestern Louisiana, in cooperation with ACM. Contact: Ralph Sproule, Jr., University of Hawaii, 2404 Maili Way, Honolulu, HI 96822. (808) 944-7430; or Bruce Shirver, Computer Science Department, University of Southwestern Louisiana, P. O. Box 40330, Lafayette, LA 70504. (318) 231-6606.

7-9 Statistical and Computational Problems in Probability Modeling. Williamsburg, Virginia. The conference will be structured around six main themes: random number generation, simulation, reliability and survival modeling, statistical inference for stochastic models, traditional and new approaches to time series modeling, real world issues in probability modeling, numerical methods in probability. Contact: Professor Carl M. Harris, Department of Systems Engineering, University of Virginia, Charlottesville, VA 22901. (804) 924-3803.

16-18 1985 BENELUX Meeting on Systems and Control. Louvain-la-Neuve, Belgium. Contact: Dr. G. Campion, Universite Catholique de Louvain, Unité AUTO - Batiment Maxwell, Place du Levant 3, B 1314 Louvain la Neuve, Belgium. (010) 418181, ext 2361.


24-26 SCS Multiconference: Modeling and Simulation on Microcomputers; Computer Simulation in Emergency Planning; Distributed Simulation; AI, Graphics and Simulation. San Diego, California. Sponsor, SCS. Contact: Charles A. Pratt, SCS, P.O. Box 2228, La Jolla, CA 92038. (619) 459-3988.

MARCH 1985

13-15 Annual Simulation Symposium. Tampa, Florida. Contact: Professor John E. Comfort, Department of Mathematical Sciences, Florida University, Miami, FL 33199. (305) 224-3015.

13-15 International Workshop on Artificial Intelligence in Economics and Management. Zurich, Switzerland. Contact: IFAC, IFORS, IFIP, MPS, and IEEE. Contact: J. P. Pau, IFAC Workshop. Battelle Memorial Institute, 7 route de Druye, CH 1227 Geneva, Switzerland.


-11-
Institut für Angewandte Informatik und Formale Beschreibungsverfahren, University of Karlsruhe, D-76128 Karlsruhe, West Germany.

27-29

31
1985 Microprocessor Forum. Atlantic City. Apr. 4

APRIL 1985

14-18

25-26

MAY 1985

2-3
End-User Computing: The Changing Role of the Systems Professionals and the End-User. Minneapolis, Minnesota. Sponsors: ACM SIGBDP (Business Data Processing) and ACM SIGCPR (Computer Personnel Research). See August Communications, 3e, of full paper with 1-paragraph abstract to: James C. Wetherbe, MIS Research Center, University of Minnesota, 269 16th Avenue South, Minneapolis, MN 55455.

13-17
Fifth International Conference on Distributed Computing Systems. Denver, Colorado. Sponsor IEEE-CS. See August Communications, 4s, of 20 pp paper with 130-word abstract to: Ming T. Liu, Ohio State University, Computer and Information Systems 2036 Neil Avenue, Columbus, OH 43210.

19-21
6th IFAC Workshop Distributed Computer Control Systems. San Francisco, California. Contact: Dr. R. W. Gellie, CSIRO, P. O. Box 71, Fitzroy, 3065, Australia.

JUNE 1985

11-13

11-14
5th IFAC Workshop on Control Applications of Nonlinear Programming and Optimization. Capri, Italy. Contact: Professor G. Di Pillo, Dipartimento di Informatica e Sistemistica. Università degli Studi di Roma "La Sapienza," Via Eudossiana 18, 00184, Roma, Italy.

19-21
1983 American Control Conference. Boston Marriott Hotel, Copley Place, Boston, Massachusetts. Contact: Professor David Warmsley, Department of Mechanical Engineering, MIT, Cambridge, MA 02139.

23-26
22nd Design Automation Conference. Las Vegas, Nevada. Sponsors: ACM SIGDA (Design Automation) and IEEE-CS. Conference cochairmen: Hillel Ofei, IBM (B2211951), P. O. Box 390, Poughkeepsie, NY 12602. (914) 465-7763.

JULY 1985

3-7
7th IFAC/FORS Symposium Identification and System Parameter Estimation. York, United Kingdom. Contact: Professor H. A. Barker, University College of Swansea, Department of Electrical and Electronic Engineering, Singleton Park, Swansea SA2 8PP, UK.

15-18

16-19

16-19
Summer Computer Simulation Conference. Chicago, Illinois. Sponsor: SCS.

22-24
Summer Computer Simulation Conference. Chicago, Illinois. Sponsor: SCS. Contact: Charles A. Pratt, P. O. Box 2228, La Jolla, CA 92038; (619) 459-3888.

22-26
SIGGRAPH '85, San Francisco, California. Sponsor: ACM SIGGRAPH. Contact: ACM Conference Management Department, 11 West 42nd Street, New York, NY 10036. (212) 869-7440, ext. 290.

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29

29

AUGUST 1985

4-8
NOVEMBER 1985

18-20 IFAC Workshop Automatic Control in Petroleum, Petrochemical and Desalination Industries. Kuwait. Contact: Dr. Janfar Assiri, c/o Dr. Samir Kotob, TED ASD, Kuwait Institute for Scientific Research, P. O. Box 21885, Safat, Kuwait.

DECEMBER 1985


JANUARY 1986


MARCH 1986


JUNE 1986


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- DuPont Committee on Educational Aid
- EXXON Research & Engineering Company
- The Halcon SD Group, Inc.
- Monsanto Fund, Monsanto Company
- Olin Chemicals Corporation
- Pfizer Foundation
- Process Simulation Int'l
- Shell Companies Foundation
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LIST OF CHEMICAL ENGINEERING DEPARTMENTS SUPPORTING CACHE

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- University of California, Santa Barbara
- California Institute of Technology
- California State Polytechnic University, Pomona
- University of Southern California
- Carnegie-Mellon University
- Case Western Reserve University
- Christian Brothers College
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- Clarkson College of Technology
- Cleveland State University
- Colorado State University
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- University of Notre Dame
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- Ohio University
- University of Oklahoma
- Oklahoma State University
- Oregon State University
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- Pennsylvania State University
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- University of Rochester
- Rutgers - The State University
- University of South Carolina
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- Syracuse University
- University of Tennessee
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- Texas A & M University
- Texas Tech University
- University of Toledo
- University of Tulsa
- University of Utah
- Villanova University
- University of Virginia
- University of Washington
- Wayne State University
- University of Wisconsin
- Worcester Polytechnic Institute
- Yale University
- Youngstown University

1982-1984

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- Auburn University
- University of California, Berkeley
- University of California, Davis
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- Clemson University
- Colorado School of Mines
- University of Colorado
- University of Connecticut
- Cornell University
- Georgia Institute of Technology
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- University of Maryland
- University of Michigan
- Michigan Technological University
- University of Minnesota
- Mississippi State University
- University of Nevada, Reno
- New Jersey Institute of Technology
- City College of New York
- University of North Dakota
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<td>University of Wyoming</td>
</tr>
<tr>
<td>University of South Florida</td>
<td>University of Waterloo</td>
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</table>
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549 East University Avenue
Ann Arbor, Michigan 48109

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and J. E. Paulse $13.95 each

No. of EXERCISES IN PROCESS SIMULATION USING FLOWTRAN, 2nd Edition,
edited by J. P. Clark,
I. P. Koehler, and
J. T. Summerfield $11.95 each

No. of CACHE USE OF FLOWTRAN ON UCS,
copies 2nd edition, by R. R. Hughes
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Address: ____________________________

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Make check payable to Ulrich's Bookstore.

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I am interested in obtaining a FLOWTRAN tape.

If you have checked either of the above squares, please complete the following information. If you have two computers you want to consider, duplicate this form, submit both completed forms and your preference.

1) Computer make and complete model number

2) Operating system version

3) FORTRAN compiler version

4) Magnetic tape facility:

   No. of tracks

   Drive speed in bits/inch

Name: ____________________________

Address: ____________________________

______________________________

Send the form to: Professor J. D. Seader
CACHE
3062 MEB
University of Utah
Salt Lake City, UT 84112

Send this form only if you have not previously contacted Professor Seader.

Name ____________________________________________

Address __________________________________________

________________________________________________

(City) (State) (Zip)

Date ____________________

Signature __________________________

Send form and remittance (or purchase order) to:

Brice Carnahan
Department of Chemical Engineering
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Ann Arbor, MI 48109

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