CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 35

Fall 1992

The CACHE CORPORATION

WHAT IS CACHE?

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

CREATION OF THE CACHE CORPORATION

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

CACHE ACTIVITIES

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

CACHE Corporation
P. O. Box 7939
Austin, Texas 78713-7939
(512) 471-4933
CACHE@UTXVM.CC.UTEXAS.EDU.

CACHE NEWS

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

CACHE NEWS

No. 35 Fall 1992

CACHE Trustees

President:
Michael B. Cutlip, University of Connecticut
(BITNET: MCUTLIP@UCONNVM)

Vice President
Ignacio Grossmann, Carnegie Mellon University
(BITNET: D391GR99@VB.CC.CMU.EDU)

Secretary
Yaman Arkun, Georgia Institute of Technology
(BITNET: YAMAN_ARKUN@CHEMENG.GATECH.EDU)

Executive Officer
David M. Himmelblau, University of Texas at Austin
(BITNET: CACHE@UTXVM.CC.UTEXAS.EDU)

Academic Trustees
L. T. Biegler, Carnegie Mellon University
(BITNET: D101LB01@CMCCVB)
Brice Carnahan, University of Michigan,
(BITNET:BRICE_CARNAHAN@UB.CC.UMICH.EDU)
James F. Davis, Ohio State University
(BITNET: KCGL1.ENG.OHIO-STATE.EDU)
Michael F. Doherty, University of Massachusetts
(BITNET: MDOHERTY@UMAECS.BITNET)
Thomas F. Edgar, University of Texas at Austin
(BITNET: UTXCHE@UTCHPC.BITNET)
Bruce A. Finlayson, University of Washington
(BITNET: FINLAYSON@CHEVAX.CHEME.WASHINGTON.EDU)
H. Scott Fogler, University of Michigan
(BITNET: H_SCOTT_FOGLER@UM.CC.UMICH.EDU)
Andrew N. Hrymak, McMaster University
(BITNET: HRYMAK@MCMASTER)
Sangtae Kim, University of Wisconsin
(BITNET:KIM@CHEWI.CHE.WISC.EDU)

Academic Trustees, continued

Richard S. H. Mah, Northwestern University
(BITNET: DICK_MAH@NUACC)
Manfred Morari, California Institute of Technology
(BITNET: MM@IMC.CALTECH.EDU)
Gintaras V. Reklaitis, Purdue University
(BITNET: REKLAITI@ECN.PURDUE.EDU)
Peter R. Rony, Virginia Polytechnic Institute and State University
(BITNET: RONY@VTVM1)
J. D. Seader, University of Utah
(BITNET: SEADER@UTAHCCA)
Warren D. Seider, University of Pennsylvania
(BITNET: SEIDER@CHEME.SEAS.UPENN.EDU)
George Stephanopoulos, Massachusetts Institute of Technology

Industrial Trustees
Gary E. Blau, Dow Chemical Company
John C. Hale, E. I. DuPont de Nemours & Co.
(BITNET: HALE@PCCVAX.DNET.DUPONT.COM)
Norman E. Rawson, IBM
(BITNET: NERAWSO@BETVMIC5.VNET.IBM.COM)
Edward M. Rosen, Monsanto Company
(BITNET: C00820ER@WUVMD)
Jeffrey J. Siirola, Eastman Kodak
(BITNET: SIIROLA@KODAK.COM)
Joseph D. Wright, Xerox
(BITNET: WRIGHT@MCMASTER)
or WRIGHT.XRCC-NS@XEROX.COM)

Advisory Committee
Lawrence B. Evans, Massachusetts Institute of Technology
James R. Fair, University of Texas at Austin
Thomas H. Lafferre, Monsanto Company
John J. McKetta, University of Texas at Austin

CACHE Task Forces and Committees

STANDING COMMITTEES

Publications
Prof. Brice Carnahan
Dept. of Chemical Engineering
University of Michigan
Ann Arbor, Michigan 48109
(313) 764-3366

Newsletter
Prof. David M. Himmelblau
Dept. of Chemical Engineering
University of Texas
Austin, Texas 78712
(512) 471-7445

Conferences
Prof. Richard S. H. Mah
Dept. of Chemical Engineering
Northwestern University
Evanston, Illinois 60201
(708) 491-5357

Curriculum
Prof. James F. Davis
Dept. of Chemical Engineering
Ohio State University
140 West 19th Avenue
Columbus, OH 43210-1180
(614) 292-2359

TASK FORCES

Artificial Intelligence
Prof. George Stephanopoulos
Dept. of Chemical Engineering
Massachusetts Institute of Technology
66-562
Cambridge, Massachusetts 02139
(617) 253-3904

Process Engineering
Dr. Edward M. Rosen
Monsanto Company - F2WK
800 N. Lindbergh Blvd.
St. Louis, Missouri 63167
(314) 694-6412

Case Studies
Professor Ignacio Grossmann
Dept. of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2228

Electronic Mail
Prof. Peter Rony
Dept. of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, Virginia 24061
(703) 961-7658

NSF Development of Innovative Engineers
Prof. H. Scott Fogler
Dept. of Chemical Engineering
3074 Dow Building
University of Michigan
Ann Arbor, Michigan 48109
(313) 764-2384

NSF Simulated Laboratory Modules
Prof. Gintaras V. Reklaitis
School of Chemical Engineering
Purdue University
West Lafayette, Indiana 47907
(317) 494-4075

Graphical Computer Aids for ChE Education
Prof. Bruce A. Finlayson
Dept. of Chemical Engineering, BF-10
University of Washington
Seattle, Washington 98195
(206) 543-2250

ChemSep - Another Software System for the Simulation of Separation Processes

By Harry Kooijman and Ross Taylor
Department of Chemical Engineering
Clarkson University
Potsdam, New York 13699-5705
USA

ChemSep is our name for a suite of programs that perform multicomponent separation process calculations. This article presents a brief description of ChemSep together with some illustrations created by the package.

Design and simulation of multicomponent separation processes such as distillation is an important part of modern chemical engineering. For about three decades now such calculations have been carried out using computer programs that attempt to solve the equations that model distillation operations, the so-called MESH equations (see, for example, Henley and Seader, 1981). The M equations are the Material balance equations, the E equations are the Equilibrium relations, and the H equations are the entHalpy balance equations. The S equations are the mole fraction Summation equations.

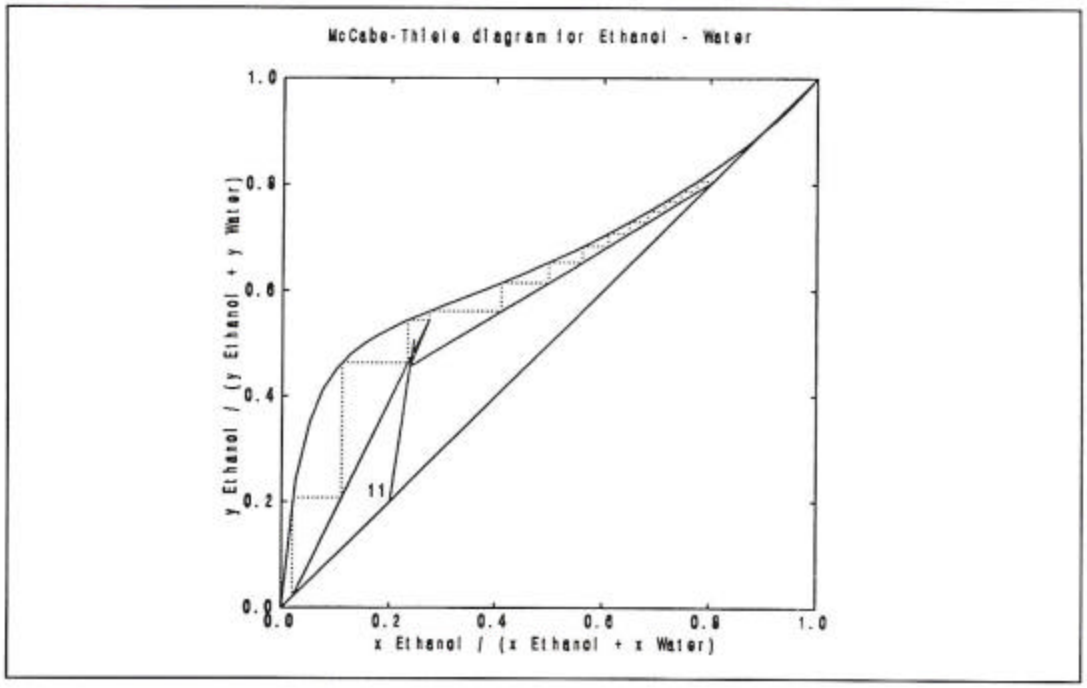


Figure 1
McCabe-Thiele diagram for distillation of ethanol-water mixture. Column has 13 stages including a total condenser and a partial reboiler.

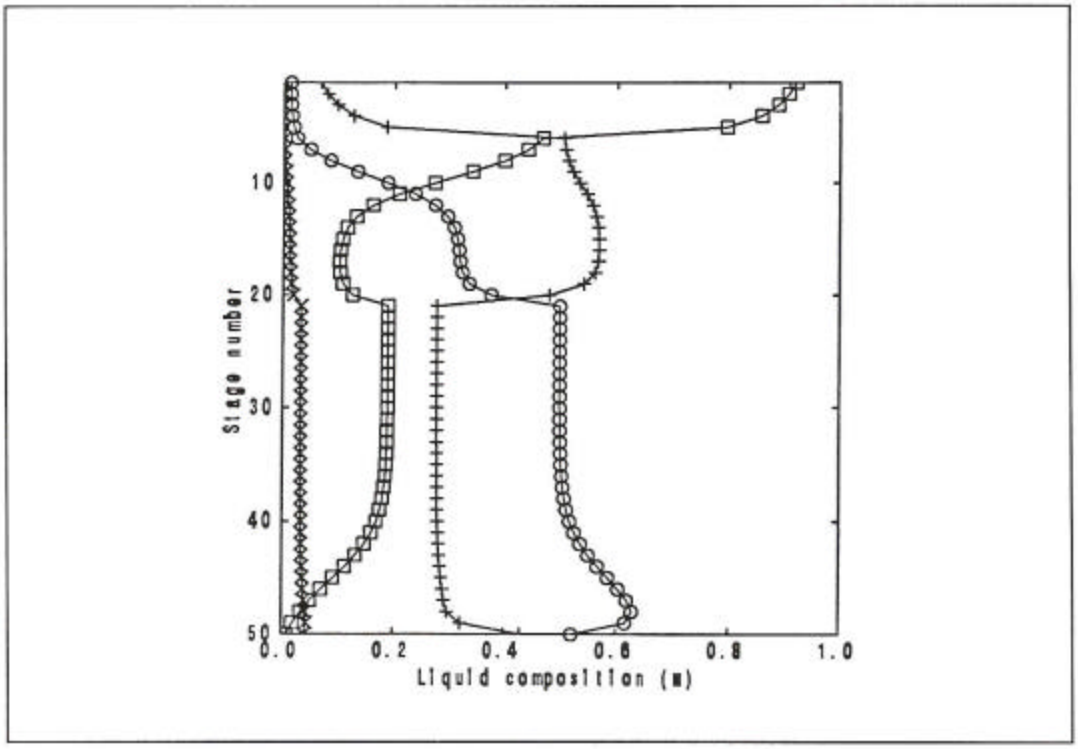


Figure 2
Liquid composition profiles for extractive distillation of acetone, methanol, ethanol, water system.

There can be few other mathematical models in any branch of engineering which are so well suited to computer solution and that have prompted the development of so many truly different algorithms. Since the late 1950s, hardly a year has gone by without the publication of at least one (and usually more than one) new algorithm (Seader, 1985). The evolution of algorithms for solving the *MESH* equations has been influenced by, among many other things, the availability (or lack) of sufficient computer storage and power. Not so very long ago a distillation column simulation had to be performed on a mainframe or mini computer. However, the remarkable increase in the capabilities of personal computers throughout the 1980s has meant that distillation columns often can be effectively simulated on such machines.

Our own interest in computer simulation in general and of distillation in particular is due in part to the fact that we find distillation calculations quite fascinating. We are involved with students who need to simulate distillation operations either as part of a course on separation processes or as part of a large scale design project that all students must do in their final year of study. In the past these design studies were performed with simulation systems that were installed on a mainframe computer.

In our view, much of the software capable of solving distillation problems that existed when we were planning *ChemSep* was not suitable for use in the first undergraduate course that deals with stagewise separation processes. For one thing, the comprehensive flowsheeting packages of the time lacked interfaces that were as easy to use and as flexible as we thought they could be. In addition, very few such programs could be run on the kinds of computers that students might possess. Finally, most such programs were not available at prices low enough for students to acquire their own copy.

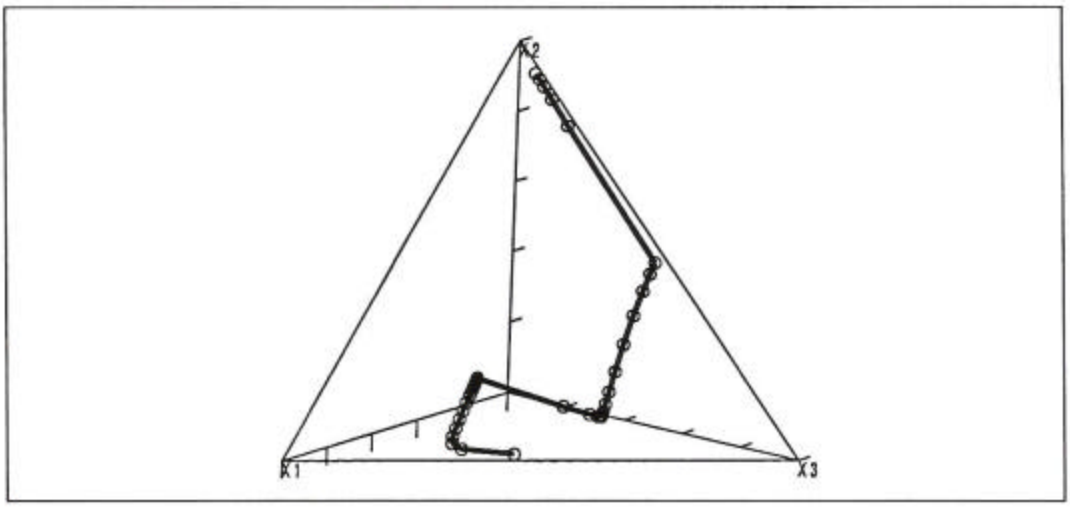


Figure 3
Quaternary diagram for extractive distillation system in Figure 2.

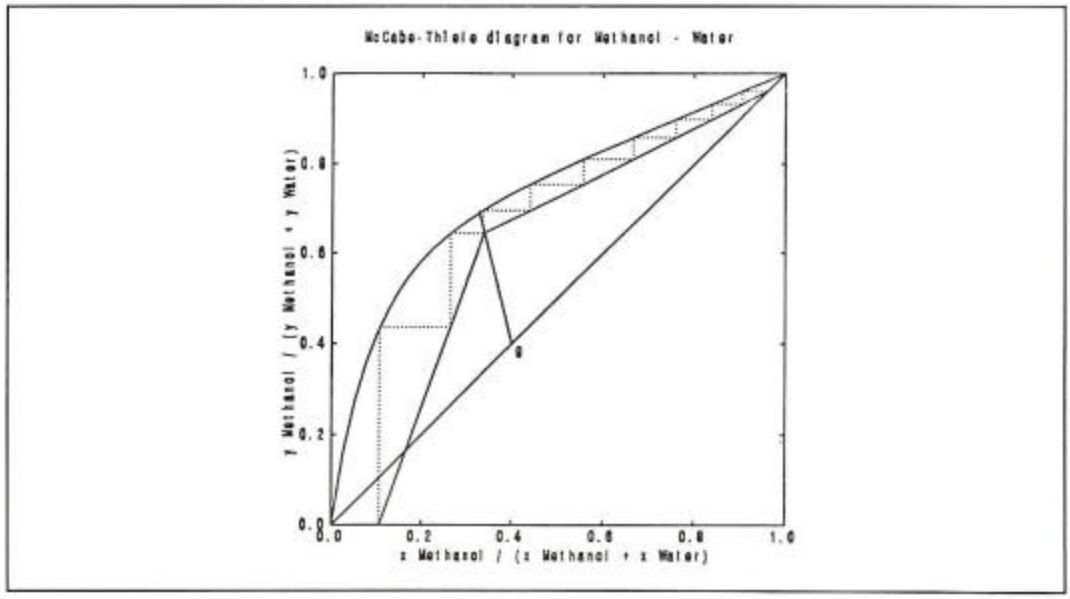


Figure 4
McCabe-Thiele diagram for separation of methanol-water mixture.
Column has no reboiler and heat is supplied by open steam.

With these (and other) thoughts in mind Arno Haket and ourselves began the *ChemSep* project in February 1988 at the University of Technology in Delft (TU Delft) in The Netherlands. Version 0.92 of *ChemSep* was first introduced to graduate and undergraduate level students at Delft in September 1988 by Professor Hans Wesselingh of the TU Delft (presently at the Rijks Universiteit Groningen in The Netherlands). The use of *ChemSep* by Professor Wesselingh in the courses he taught was of enormous value to us in improving the programs.

As a result of the success enjoyed by the program during those first courses at Delft, we continued to develop *ChemSep*. A series of improved versions (numbered 1.0 to 1.5) was developed by Arno Haket and Harry Kooijman in Delft and Ross Taylor in Potsdam, New York. This development would have been difficult if it were not for the international computer networks that allowed us to hold intercontinental computerized conversations and exchange working programs. Many pages of electronic mail testify to our progress (and lack of progress) over the last few years. We find it interesting to look back on our mail and discover the things that we argued about so long ago in our efforts to make things "just right".

In March 1991 we began writing *ChemSep* 2.0. This version is a completely new set of programs and data files with many new and improved features. Version 2.0 was first used in courses at the University of Amsterdam and at Clarkson University in Potsdam, New York in September 1991.

Some of the features of the *student edition* of *ChemSep* 2.0 are identified in Table 1.

Features of Student Edition
Interactive interface with menus/spreadsheets/windows
Equilibrium flash calculation program
Equilibrium column simulation program
A wide variety of thermodynamic models (see Table 2)
Library of physical property data for 189 components
Advanced component selection procedures
(recursively by name, formula, structure, property value and more)
Extensive context sensitive (hypertext-like) help system
On line technical background
Data entry can include algebraic calculations and units
Unit conversions
Automatic checking for missing input
Degrees of freedom analysis
Warnings for difficult specifications
Composition, flow, temperature, and stripping factor profiles displayed graphically
Key ratio diagrams
Profiles can be mixed on the same diagram
McCabe-Thiele diagrams (even for multicomponent systems)
Right triangular diagrams (for three or more components)
Tetrahedron diagrams for 4 component systems (can be rotated)
Graphs are fully configurable (line and point style, color, etc.)
Tabular output can be edited, then printed or saved in a text file
Spreadsheet files can be printed in ASCII text or Lotus WK1 formats
Many printers/plotters/desktop publishing formats supported (see Table 3)
Macro language
Built in file viewer and text editor
Mouse support
System Requirements
IBM PC or PC compatible using DOS 3.0 or higher
640 kB total RAM memory
1 MB disk space
Hard disk very strongly recommended but not required
Math coprocessor recommended but not required

Table 1
ChemSep Features and System Requirements

One of the requirements for any program like *ChemSep* is to have a built-in collection of methods for estimating thermodynamic properties. A list of property models incorporated into *ChemSep* is provided in Table 2.

K-value Models	Enthalpy
Raoult's law Equation of State Gamma-Phi DECHEMA Chao-Seader Polynomial	None Ideal Ideal + Excess Polynomial
Equations of State	**Activity Coefficients**
Ideal gas law Virial Redlich-Kwong Soave-Redlich-Kwong (SRK) API-SRK Peng-Robinson	Ideal solution Scatchard-Hildebrand (+/-Flory-Huggins) Margules Van Laar Wilson NRTL UNIQUAC UNIFAC
Vapor Pressure	
Antoine Extended Antoine DIPPR polynomial Reidel Lee-Kesler	

Table 2
Thermodynamic and Physical Property Models

ChemSep was created specifically to be useful in university courses on stagewise operations but can be (and is) used by professional engineers in industry. The software has also been used in undergraduate and graduate courses on thermodynamics and design. The software was designed to be easy to use by students with no experience of engineering software while having sufficient flexibility and power to appeal to expert users. In pursuit of these objectives *ChemSep* features a menu-driven, user-friendly interface with an integrated help system and an autopilot mode that leads the novice user through the data input phase. Expert users, however, are not forced to follow the path taken by the autopilot but can proceed to enter data in any order they wish. *ChemSep* allows users to assign special functions to certain key combinations and this can be of considerable help in developing a personal, more efficient way of working within *ChemSep*.

ChemSep runs under DOS 3.0 or higher with 640 kBytes of installed RAM memory. The total disk space required is around 1 Mbyte for a basic *ChemSep* setup. However, if you install all the video and printer drivers you will need about 2 Mbyte. *ChemSep* can be run from floppy disks but we do not recommend that. *ChemSep*'s interface and calculation programs are entirely separate and are loaded into memory as needed. This takes some time to accomplish from a floppy disk-based system. A math-coprocessor is not required but *ChemSep* will use it of one is present in the computer. If nothing else, running a distillation simulation on a machine with no coprocessor will make you wish that you had one.

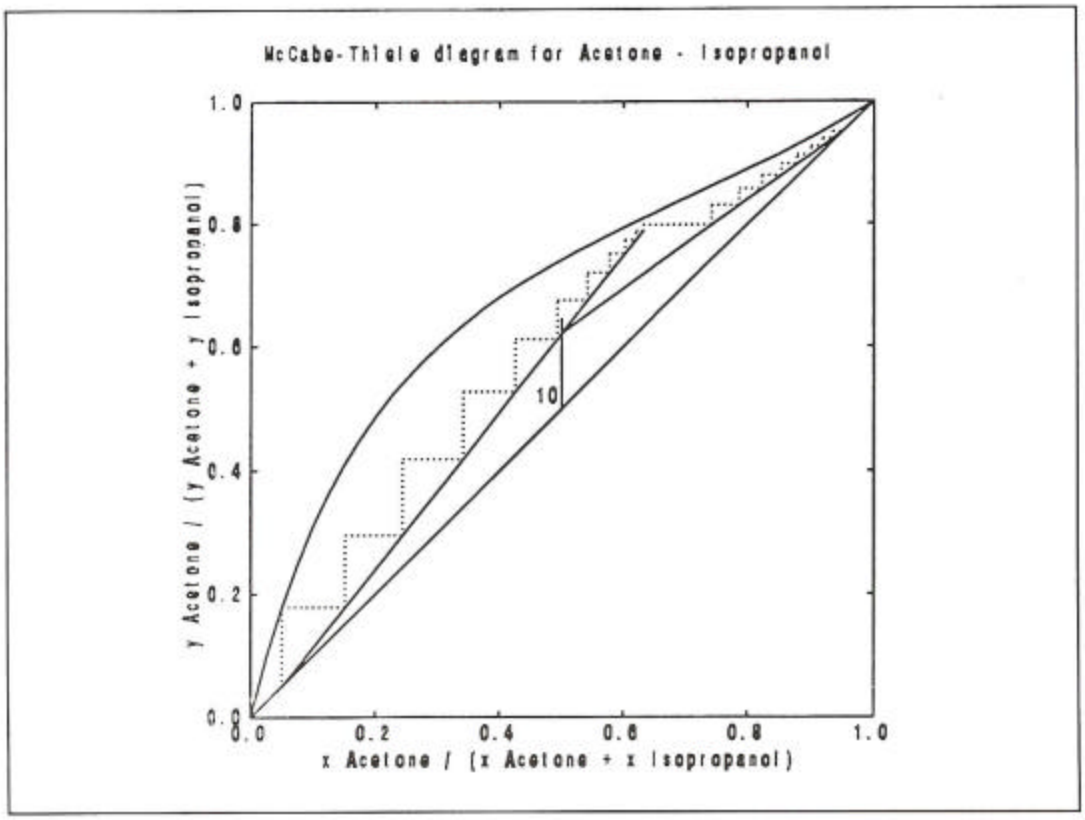


Figure 5
McCabe-Thiele diagram for distillation of acetone - isopropanol mixture. Note the use of specified Murphree efficiencies and the poor location of the feed stage.

Tables of results are displayed in a window that can be edited before directing the output to a file or to a printer. Graphs are completely configurable by the user. *ChemSep* supports many different output devices as shown on the following page in Table 3. *ChemSep* can also print graphical output in several different graphics formats used by desktop publishing or major word processing software packages (see Table 3 again). The illustrations that accompany this article were printed in Word Perfect Graphics format, imported into the word processor of that name and printed with no further editing.

ChemSep 2.0 is the result of too many hours of coding, testing and recoding in our "free" time. It consists of four executable files plus a number of small data files for recording various bits and pieces of information. The driver and interfaceare written in Turbo Pascal (version 5.5) and involve around 30,000 lines of code. The flash and column simulation programs (FLASH2 and COL2) are written in standard Fortran 77. The source code is approximately 25,000 lines in length. The code has been developed on Zenith Z-248 and Z-386 microcomputers with the help of the F77 and F77/386 compilers (versions 8.5) from WATCOM. The source code for the column and flash calculations has also been successfully compiled (unchanged) and executed on DEC VAX computers and on Sun Workstations.

Printers/Plotters Supported	Desktop Publishing File Formats
Epson 9-pin dot matrix Color Epson 9-pin dot matrix Epson 24-pin dot matrix Color Epson 24-pin dot matrix IBM Proprinter X24 IBM Quietwriter Toshiba 24-pin dot matrix Okidata ML-92 dot matrix LaserJet II LaserJet III DeskJet Color DeskJet PaintJet Postscript Hewlett-Packard 7090 Hewlett-Packard 7470 Hewlett-Packard 7475 Hewlett-Packard 7550 Hewlett-Packard 7585 Hewlett-Packard 7595	ZSoft PCX Windows 3 BMP GEM IMG TIFF compressed TIFF uncompressed ANSI CGM AutoCAD DXF Video Show Word Perfect Graphics

Table 3
Output Devices Supported by *ChemSep*

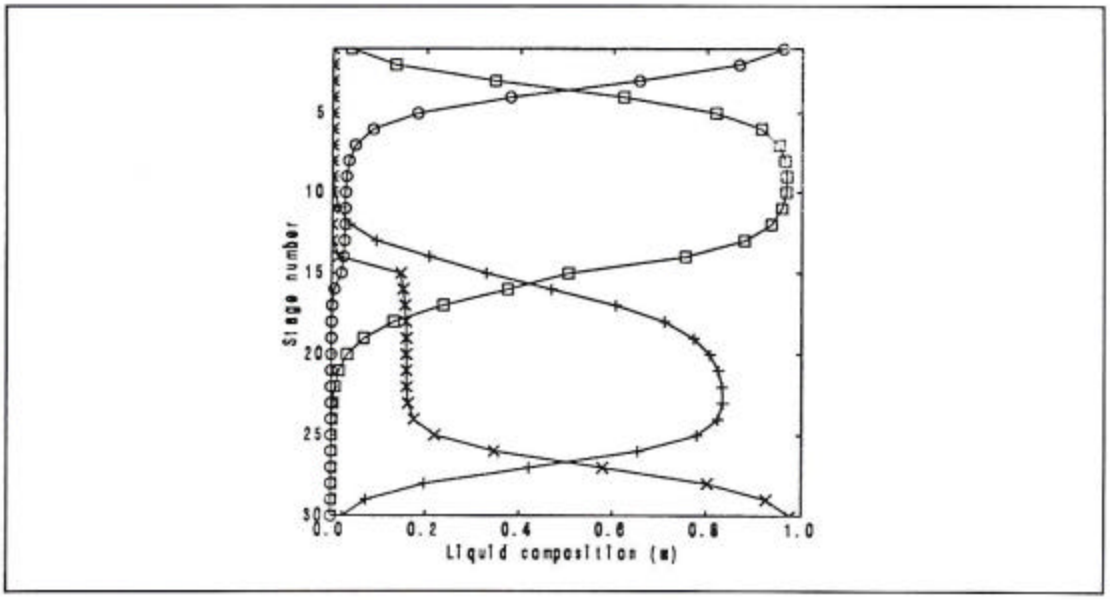


Figure 6
Composition profiles in the distillation of n-Butane, n-Pentane, n-Hexane, and n-Octane. Column has 30 stages, feed to 15, sidedraws from 10 and 24..

The numerical method used in COL2 and FLASH2 to solve the model equations is a simultaneous correction method in which all of the equations are solved simultaneously using Newton's method. Simultaneous correction methods require the partial derivatives of all equations with respect to all variables. This means evaluating the partial derivatives of thermodynamic properties with respect to composition, temperature and pressure. All partial derivatives, with the exception of the temperature derivative of excess enthalpy, are computed analytically.

We try to improve the *ChemSep* software as time permits and updates of our software will appear on a regular basis as new features are added. Next year, for example, there will be a significant new release with the addition to *ChemSep* of a model based on mass transfer principles, the nonequilibrium model of Krishnamurthy and Taylor (1985). We welcome suggestions for new features and improvements and will try to incorporate as many new ideas as possible.

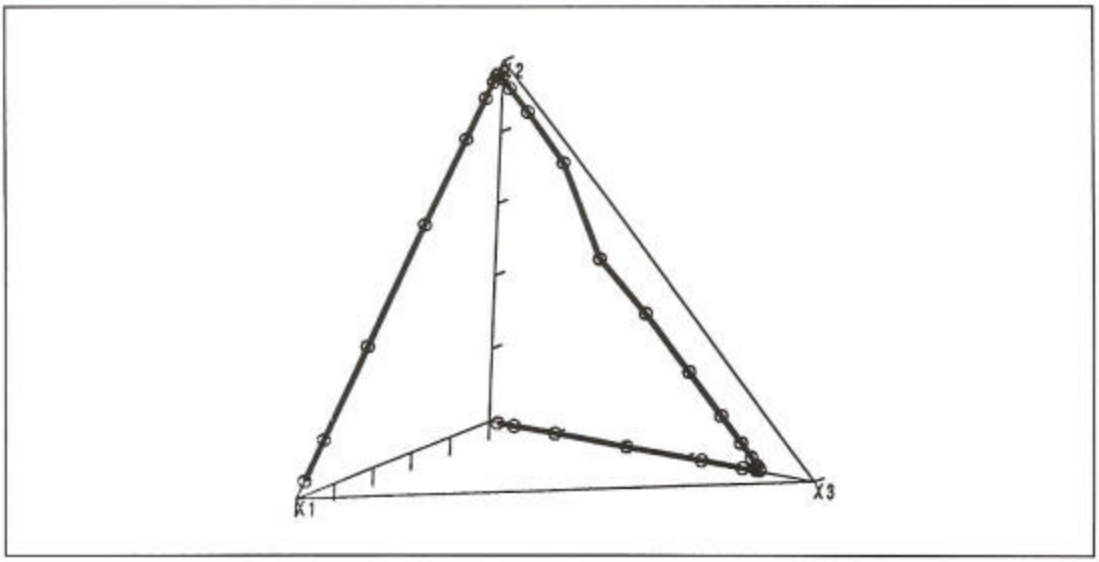


Figure 7
Quaternary diagram for distillation of n-butane, n-pentane, n-hexane, and n-octane. The example is based on Exercise 15-28 in the textbook of Henley and Seader.

Acknowledgments

Our thanks above all go to Arno Haket. Arno was an essential part of the team that created the early versions of *ChemSep*. Our thanks also to Professor Hans Wesselingh and Peter Verheijen and to many friends and colleagues at universities in The Netherlands and in the USA who have used earlier versions of *ChemSep* in their courses or who have tested the program for us. Last, but not least, our thanks to the many students on both sides of the Atlantic Ocean that were forced to use this program or risk failing one of their required courses.

Most of the illustrations that accompany this article are inspired by exercises or examples in the textbooks by P.C. Wankat (1988) (Figures 1 and 4) and by E.J. Henley and J.D. Seader (1981) (Figures 5-7). Additional illustrations of the use of *ChemSep* are presented in the Users Guide and in the Case Book.

References

Henley, E.J. and J.D. Seader, Equilibrium Stage Separation Operations in Chemical Engineering, Wiley, 1981.

Krishnamurthy, R. and R. Taylor, A Nonequilibrium Stage Model of Multicomponent Separation Processes: I. Model Description and Method of Solution, A.I.Ch.E. J., 31, 449-457, 1985.

Seader, J.D. The B.C. (Before Computers and A.D. of Equilibrium Stage Operations, Chem. Eng. Ed., XIX(2, Spring), 88-103, 1985.
Wankat, P.C., Equilibrium Staged Separations, Elsevier, 1988.

The Authors

Harry Kooijman is a PhD candidate at Clarkson University. His research work is concerned with developing dynamic models of separation processes based on mass transfer principles. His prior degree is from the Technical University Delft (TUD).

Ross Taylor is a Professor of Chemical Engineering at Clarkson University. His research and teaching interests center around separation processes, mass transfer and design.

Notices

WATCOMF-77 and F-77/386 are products of WATCOM Inc. Turbo Pascal is a product of Borland International Inc.

Anonymous FTP Servers

By Sangtae Kim, University of Wisconsin

Anonymous FTP servers have become a popular vehicle for distributing a host of products, from public domain software and shareware, to reprints of technical reports. This article provides a brief introduction suitable for the typical user. Issues such as how to set up an anonymous FTP server will not be addressed.

Readers may already be acquainted with FTP (file transfer protocol) available as part of the Unix operating system. A user with accounts on two different Unix computers (let's call them **here** and **eternity**) may transfer a file from **here** to **eternity** by first logging on to **eternity** and typing:

```
ftp here
Name (eternity:prue): prue
231 Password required for prue
Password: prue's-password
230 User prue logged in.
ftp> get taps.memo
200 PORT command successful.
150 Opening ASCII mode data ...
226 Transfer complete.
local:  taps.memo remote:  taps.memo
20577 bytes received in 0.07 seconds ...
ftp> bye
```

In the above example, the computer prompts are denoted with typewriter fonts, while user inputs are in italic fonts.

The essential idea of *anonymous* ftp is that the user accounts and passwords are not required. The user's account is replaced by the generic account name *anonymous*. The following example illustrates how anyone on the Internet network may obtain a copy of the errata sheet for *Microhydrodynamics*. Again, the two fonts differentiate computer prompts and user input.

```
ftp doug.cae.wisc.edu
Connected to doug.cae.wisc.edu.
220 doug FTP server ... ready.
Name (doug.cae.wisc.edu:stkim): anonymous
331 Guest login ok, send ident as password.
Password: anything-preferably-your-name
230-User ftp: working directory set to ...
230 Guest login ok, access restrictions
   apply.
ftp> cd pub/microhydro
200 CWD command okay.
ftp> get errata.txt
200 PORT command okay.
150 Opening data connection for errata.txt
   ...
226 Transfer complete.
local:  errata.txt remote:  errata.txt
4611 bytes received in 0.082 seconds ...
```

Here are two more illustrative examples:

```
ftp nic.ddn.mil
Connected to nic.ddn.mil.
220-Welcome to the Network Information
   Center
Login with... 'anonymous" and password
   "guest"
You may change directories to the follow-
   ing:
ddn-news - DDN Management Bulletins
domain - Root Domain Zone Files
iesg - IETF Steering Group
ietf - Internet Engineering Task Force
internet-drafts - Internet Drafts
netinfo - NIC Information Files
netprog - Guest Software (ex.  whois.c)
protocols - TCP-IP & OSI Documents
rfc - RFC Repository
scc - DDN Security Bulletins
std - Internet Protocol Standards
220 And more!
Name (nic.ddn.mil:stkim): anonymous
```

and so forth.

Our third example retrieves the list of PYI Awards for 1991 from the NSF anonymous ftp server.

```
ftp stis.nsf.gov
Connected to stis.nsf.gov.
220 stis.nsf.gov FTP server ...
Name (stis.nsf.gov:stkim): anonymous
331 Guest login ok,
send your E-Mail address as password.
Password: put-your-email-address-here
```

```
230- Guest login ok, access restrictions
   apply.230 Welcome to the STIS System
ftp> get pyi91
200 PORT command successful.
150 Opening ASCII mode data connection ...
226 Transfer complete.
local:  pyi91 remote:  pyi91
31775 bytes received in 1 seconds ...
ftp> bye
```

The filename pyi91 was determined by applying the Unix 'ls' command to get a listing of all the files (there are lots of files in all) in the directory.

There are now literally thousands of anonymous ftp servers in the USA and beyond containing a veritable smorgasbord of software packages: plotting routines, 3-D graphics and visualization packages, spreadsheets, symbolic algebra programs, compilers, desktop publishing software, and yes, even some nifty games. The only way to keep track of them is with the help of (what else?) anonymous ftp servers!

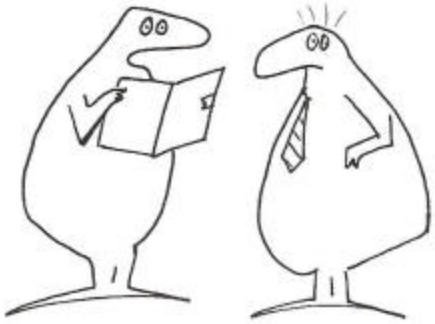
Readers may search and retrieve a particular software package using the archie program (developed by Alan Emtage and Perter Deutsch of McGill University) to query a central database that contains the contents of all known anonymous ftp servers. For example, to track down the availability of the gnuplot plotting package, type:

archie -h archie.unl.edu gnuplot

on your computer. The machine at the University of Nebraska - Lincoln will return a list of ftp servers that have gnuplot distribution sets. The archie program itself is available from archie.unl.edu *by anonymous ftp server!*

Acknowledgement

I would like to thank Douglas Brune for his contributions to this article.



The good news is you can send electronic mail to 1000 chemical engineering professors instantaneously. The bad news is that they can do it to you.

Name Servers: or Electronic Mail Made Easy

By Sangtae Kim
University of Wisconsin

Name servers are used to map host names to host addresses on the Internet. They are also used to map host addresses to host names and to route electronic mail. Perhaps the following summary of life before name servers best illustrates their utility.

There are those who embrace electronic mail and wonder how life was possible before it was invented, and those who refuse to open yet another channel of communications (claiming that they already get too much 'regular' mail). Somewhere in the middle are the masses that see the merit of electronic mail and would even use it occasionally, but are scared away by the formidable routing protocols.

Before name servers came into widespread usage, senders had to give the routing from source to destination computers, with the details depending on the mail protocol employed (see the Fall '89 and Spring '90 issues of CACHE News). It was not unusual for addresses of international colleagues to take up the entire line (80 characters). For example, during the period 1988-90 when I was writing Microhydrodynamics, my electronic mail to my co-author Seppo Karrila had to be addressed as: `@bossie.macc.wisc.edu:@cunyvm.cuny.edu:X@Y.abo.fi`. This routing told my computer to send the message to the Vax at the Madison Academic Computer Center, which would then forward it to cunyvm, a major gateway machine at the City University of New York. This machine would see to it that the message was delivered to the appropriate computer at Åbo Akedemi in Finland. Note that in addition to knowing the username ('X') and name/address of the destination computer ('Y'), the sender had to specify two gateways. When I update my .hosts table (discussed below) on my workstation with the ip number for cunyvm, I was able to shorten this to: `@cunyvm.cuny.edu:X@Y.abo.fi`.

Even maintaining a 'domestic mail' link between Unix workstations on the Internet system was quite arduous. The workstation owner (or at least his or her graduate students) had to maintain a 'hosts' table with the ip name and number of each destination computer. For example, during the period 1986-90, my workstation appeared in hosts tables as: 128.104.170.10 flossie.che.wisc.edu. The number 128 identifies the country (USA), 104 the institution (University of Wisconsin), 170 the campus building, and the last number identifies a particular computer. The ip name in reverse order specifies the networktype (edu), the institution (wisc), the department or subunit (che) and the name of the computer (flossie). If a friend called to announce his or her new electronic mailbox, either the hosts table had to be updated with this new information, or themessaged had to be routed through a gateway machine (which hopefully had an up tho dade hosts table).

Numbers an dnames would change frequently for various reasons including:

- Proliferation of new computers and removal of obsolete computers.
- Movement of computers from one building to another.
- IP name changes (changed boyfriend or girlfriend).

Only dichard computer hackers would have the time and energy to keep such communication lines up to date.

Name servers based on hierarchical names were proposed in the early 1980's when it became clear that a single host table would be too large to be practical. the first complete protocol specification was published in November, 1983 (RFC 883). RFC stands for Request for Comments. This is a series of documents that describes the Internet protocols, among other things. They are available with anonymous FTP from nic.ddn.mil. (See the article on anonymous FTP servers). Name servers were operational by 1986. In January, 1992, 727,000 hosts were counted in the domain name system (RFC 1296).

The hierarchical name structure allows the maintenance of the names to be divided by several sites. For example, from my viewpoint at the University of Wisconsin-Madison: the EDU domain is maintained by the Network Information Center in Virginia, WISC.EDU is maintained by the Madison Academic Computer Center ant the Computer Sciences Department, and the College of Engineering domains are maintained by Computer Aided Engineering (College of Engineering computer center). There are several name servers on the Madison campus. Each server can answer a query about any name, although it may have to query other servers to find the data. All I have to know is that the two servers in the College of Engineering are 128.104.41.30 and 128.104.38.25.

The bottom line is that, today, when I send internet electronic mail the addresses are of the form:

username@machine.dept.inst.domain

where domain is: edu within the USA or au, de, fi, jp, kr, uk, ,...(Australia, Germany, Finland, Japan, Korea, United Kingdom, ...), while for BITNET mail, the name servers will understand: username@machine.bitnet.

Acknowledgement

I would like to thank Bruce Orchard for his contributions to this article.

Process Simulation in the McMaster Curriculum

By Andrew N. Hrymak and James M. Dickson
McMaster University

The effective use of computers, especially microcomputers, is now a required skill by the chemical process industries. The curriculum issue has changed from whether students need to learn computing skills to how best to incorporate computer tools into the undergraduate chemical engineering curriculum (Denn, 1986; CACHE Corp., 1986). At McMaster, our courses use programming (Pascal or Fortran) and encourage the use of spreadsheets and wordprocessing packages. Woods (1992) has reviewed the McMaster curriculum and the philosophy behind the curriculum decisions we have made. The McMaster Problem Solving methodology runs from the sophomore through the senior years (Woods, 1990; Woods, 1991). In parallel with the open-ended problem solving/self-directed learning approach, we are developing the use of the different computer software tools through the programme.

One of the most powerful computer tools chemical engineers use on a routine basis is the process flowsheet package. Traditionally, the use of executive packages for process flowsheet simulation (such as PROCESS, ASPEN, HYSIM) is left to the senior year design project. The students are asked to learn about the process, ask questions about what should be an open-ended design question and at the same time learn about the tools that are available to help solve the subproblems they will encounter. The design course is expected to achieve many educational objectives. Instead, we have opted to meet the computer literacy objective in the earlier years of the programme. The goal is simple - students must come to think of spreadsheets and flowsheeting packages as additional tools in their toolbox of techniques to solve problems. Students must learn when process simulators should be applied, how to formulate questions, and how to evaluate whether a computed answer is reasonable. The effective use of a commercial flowsheeting package requires time and experience.

Mass and energy balancing packages have been used in our curriculum for many years beginning with GMACS. Until recently, the flowsheet packages were used in a centralized mainframe/batch mode form. Students would prepare input files, submit the job and wait (sometimes for a long time) for results. Large computer outputs would be generated and the entrails of the simulation examined for guidance about the next run. There would always be a next run. Microcomputers became widely available to the students and we decided to make the switch to a PC-based software package (Edgar, 1990). After considerable evaluation, we decided to use HYSIM (Hyprotech) beginning with the sophomore year mass and energy balancing course and continuing through the senior design course.

There are different levels of expectation for each year in the programme about the types of problems that the students are expected to handle.

Sophomore Year

Courses - Steady state mass and energy balances in chemical processes I and II

Recently the computer component (1 unit of 3) of a combined problem solving/computer skills course was shifted into the introductory chemical engineering principles course. The linking of tutorial and assignment problems to computer tools prepares the students in the use of computers for operations analysis and in the design of new systems. For some processes, programming code models are used, but engineers prefer to work with user-friendly environments such as spreadsheets and flowsheet packages. It is important for students to be able to solve problems analytically and by computer to reinforce the basic concepts but avoid the drudgery of repetitive calculations for further analyses.

During the term, there are 13 three hour tutorials. Four tutorials require the use of HYSIM. The objective is to generalize a problem already solved by hand so that many related problems could be solved. Student groups are given specific variables that they must vary and are required to use fundamentals to interpret the results.

Example Problem

From a reactor 100 kmol/h of pure n-decane comes out at 2500 °C and 33 atm pressure (absolute pressures are used). The hot gas is mixed adiabatically with 10 000 kmol/h of steam at 200 °C and 10 atm to produce a humid gas stream at 10 atm. What is the final outlet temperature? Vary the inlet temperature and pressure of the hot gas and the flow rate of the steam. Tabulate (or graph) your results of the outlet temperature as a function of the above variables.

Comments:

After considering using a spreadsheet, the students realize that they have limited thermodynamic data for these high

temperatures and pressures and they turn to HYSIM. With only a brief introduction to HYSIM, the students were running the program with little difficulty. The students used the worksheet features of HYSIM to their advantage and were easily able to move between the various HYSIM modes of operation. Students annotated their PFD (process flow diagram) with information on variables.

Example Problem

Use HYSIM to aid the design of a Vapour Compression Refrigerator operating with working fluid R-12. The compressor, operating with 100% efficiency, takes in a saturated vapour feed at -38oF and discharges at 128oF. The condenser and evaporator operate isobarically and the outlet of the condenser is a saturated liquid. An isenthalpic throttle valve closes the cycle. List the thermodynamic properties of the cyclic and the mass flow of refrigerant required and the coefficient of performance. Examine the change in the coefficient of performance by changing the following variables (assigned to individual groups): pressure drop in the evaporator, compressor inlet pressure, load on the evaporator, change to R-22 refrigerant, compressor efficiency, compressor outlet pressure, pressure drop in the condenser.

Comments:

This tutorial was used as a bonus question on an assignment. The task was to design a vapour compression refrigerator on HYSIM and then vary independent variables to see the effect on the performance of the cycle. Students learned the importance of degrees of freedom as they applied different specifications. For instance, the flow rate of refrigerant remains the only unknown until the energy load on one of the units condenser, evaporator, or compressor) is specified.

A tutorial manual for computer instruction is being prepared with 13 computer tutorials, four of which use HYSIM, for the sophomore courses.

Junior Year

Courses - Simulation, modelling and problem solving Mass transfer and stagewise operations

Students receive considerable exposure to HYSIM in a junior year course combining simulation and modelling with problem solving. They are also exposed to numerical methods in a junior year course that emphasizes model building and the appropriate use of numerical methods.

The course objectives for process simulation are:

1. To be able to convert a real process flow diagram into a form compatible with a computer executive program.
2. Given a process to be studied in the course, to be able to explain from fundamentals why the process works.
3. To be able to complete a computer simulation or design study for processes to be studied in the course.
4. To be able to integrate the fundamentals from mass and energy balances, thermodynamics, heat transfer, mass transfer and reaction kinetics/reactor design into a systems understanding of processes.
5. To summarize in writing and verbally the results of activities in this course.

These objectives are done in parallel with problem solving activities, which include: asking questions, broadening perspectives, decision-making, group skills, and time project management.

Example Case Study:

This exercise will involve the simulation of the fractionation plant for a styrene process based on the dehydrogenation of ethylbenzene. [Feed data, material costs and product purity data are provided.] Three separation schemes are examined by the groups (one scheme for each group):

Scheme I

B	B	B
T	T	T
EB	EB	
S		
α	S	
	α	

Scheme II

B	B	
T	T	T
EB	EB	EB
S		
α	S	
	α	

Scheme III

B	B	
T	T	
EB		
S		
α	EB	
	S	S
	α	α

Exercise I

Use the given feed and required product specifications, for the scheme that has been assigned to your group, to

determine:

- *i) number of theoretical trays, reflux ratio, mass and energy balances, temperatures and pressures for each column in the scheme*
- *ii) energy cost per kg styrene product producedusing rigorous column models in HYSIM for each of the units. Plot temperature, flow, and composition profiles for the stage-wise variation within the columns.*

Exercise II

Two key operating variables for improving performance are: column operating pressure and reflux ratio. For the EB/S column in your scheme, do a parameter study varying the pressure and reflux ratio to determine the effect on energy cost per kg styrene product. The perturbation in pressure and reflux ratio should still keep the plant producing products within the product requirements.

In the mass transfer course, students are exposed to more complicated distillation problem statements.

Example Problem

Consider the distillation column to separate n-hexane and toluene. The feed is 100 kmol/h at a pressure of 0.5 atm and temperature of 63.5776 °C (saturated liquid). The feed composition is 0.40 mole % n-hexane and 0.60 mole % toluene. The overhead product is specified at 43.2 kmol/h liquid (total condenser) at a pressure of 0.50 atm. The reflux ratio for the column is 3.88. The bottoms product pressure is specified to be 0.55 atm. The column has 6 ideal plates with the feed at plate three (from the top).

Examine the effects of changing the following variables: feed tray location, feed temperature, number of stages, overhead product flow rate, reflux ratio. Change each of the variables over a reasonable range to see the influence the output. Record the output variable and discuss the effect of the input variables on the output variables.

New assignments are being prepared for the junior year thermodynamics course using the extensive thermodynamics library features within HYSIM.

Senior Year Courses - Separations Chemical plant design Research project

Further problems are studied using HYSIM in the senior separations course and in the design and research project courses. By this stage, the students are comfortable with the simulation package and are able to devote more time to concentrating on the design problem. Teams of students tackle projects for external "clients". For example, in 1990-91, the client was Esso Texaco Nanticoke Refinery. The goal was to assess the effectiveness of the current wastewater treatment facility and recommend changes in the operation given strict new effluent regulations.

Summary

We have found that the students really enjoy using HYSIM. It is important to introduce the simulation package as early as possible in the curriculum so that students will appreciate the strengths and limitations of the computer tools. HYSIM can be used to enrich most of the concurrent sophomore and junior year chemical engineering courses. We continue to develop case studies based on textbook problems as well as from industrial data provided by industrial colleagues.

Acknowledgements

The efforts in curriculum development described here are due to the contributions of all our departmental colleagues. Special thanks to Dr. Cameron Crowe, Dr. Donald Woods and Dr. Philip Wood who initiated many of the curriculum changes and continue to work with us on courses that develop the students' computer skills for problem solving.

References

CACHE Corp., "Expectations of the Competence of Chemical Engineering Graduates in the Use of Computing Technology, Chemical Engineering Education, 20, 1(19), 1986.

Denn, M.M., "Design, Accreditation, and Computing Technology", Chemical Engineering Education, 20, 1(18), 1986.

Edgar, T.F., "CACHE Survey of PC-Based Flowsheet Software", CACHE News, 30(32), 1990.

Woods, D.R., "Self-Directed Learning", MPS Unit, McMaster University, Hamilton, Ontario, Canada, 1990.

Woods, D.R., "Implementing Self-Directed, Problem Based Learning in a Traditional Curriculum," Chapter 4 in The Challenge of Problem Based Learning by D. Boud and G. Feletti, Kogan Page, 1991.

Woods, D.R., "Ideas about Curriculum", Chemical Engineering Education, 26, 1(34), 1992.

More information on HYSIM is available from Hyprotech, #400, 119 - 14th Street N.W., Calgary, Alberta, Canada T2N 1Z6, Tel. (403) 283-7710.

Microcomputer Chemical Engineering Programs (developed by Professors)

Edited by Bruce A. Finlayson, University of Washington

Have you wondered what microcomputer programs are being used in other chemical engineering curricula? This column provides a mechanism for University professors to let others know about the programs they've developed and are willing to share on some basis.

The program should be described by a 250 word description, machine requirements, and ordering information. These programs should be ready to be shipped out the door, and should have been tested by students at more than one University. It would be helpful if the specific Chemical Engineering course were identified in which the program is useful. The programs will not be reviewed by Professor Finlayson, nor will they be certified by CACHE.

In order to edit the column efficiently, the submissions must be made to Finlayson via BITNET, address FINLAYSON@MAX or on a diskette in ASCII. He will acknowledge receipt of the submission via BITNET and will send the edited column to the CACHE office via BITNET. Letters cannot be accepted.

The column can only be successful if professors submit their writeups. Let us hear from you!

EZPlot, XY - Turbo Pascal Units (Libraries) for developing graphical Chemical Engineering Applications.

Dr. James P. Henley Jr.
Auburn University

EZPlot is a graphics unit for plotting functions and data (a unit is like a subroutine library, but much more powerful). XY is a unit for fitting experimental data. EZPlot was developed as a simple, yet powerful tool for visualizing two dimensional numeric data, functions and calculations, and is used in the freshman Chemical Engineering computer course at Auburn. Students quickly learn to write Turbo Pascal programs to graph functions and data. Programs written in Turbo Pascal using the EZPlot unit will run on any IBM compatible computer with CGA, MCGA, EGA, or VGA graphic systems.

XY was developed for binary vapor liquid equilibrium calculations in Unit Operations and Thermo II. The primary procedure in the XY unit is called fit_data and is called in one statement:

```
fit_data('ethanol.dat');
```

The procedure opens the data file "ethanol.dat", does a curve fit of the data, and produces two functions, Xe(y) and Ye(x). In a McCabe Thiele Distillation program, for example, the equilibrium curve, Ye(x) can be drawn by the EZPlot procedure draw:

```
draw(Ye);
```

And in the stage to stage calculations, each time the vapor composition (x) needs to be calculated from the vapor composition (y) on the same tray, the Xe function can be called:

```
x:= Xe(y);
```

When used together, EZPlot and XY allow a wide range of Chemical Engineering Problems to be solved with very short Turbo Pascal Programs. For example, a program that does a graphical McCabe Thiele solution using experimental VLE data is only 70 lines. Other programs written by the author using these units include graphing partial molar properties, liquid extraction, multi-stage batch distillation, VLE diagrams from Benedict-Webb-Rubin, Redlich-Kwong, Wilson, Van Laars, and Margules.

More information can be obtained from:

Dr. James P. Henley Jr.
Dept. of Chemical Engineering
Auburn University
Auburn University, AL 36849
INTERNET: henley@eng.auburn.edu
FAX: 205 844 2063

UC SIGNAL: Graphical Configuration of Multiloop Control System Signals

Prof. Alan Foss

Students can quickly "sketch" links between measured and manipulated variables, insert controllers and other system elements, and set tuning parameters for controllers, feedforward elements, and decouplers. Their system structure is overlaid automatically on the screen on top of a process diagram prepared by the instructor. System building is accomplished easily through mouse-directed commands to make links, to insert, move or remove elements, to interrogate connectivity, and to display and/or modify parameters associated with process elements. Control systems can be configured both for laboratory apparatus and process simulations. The completed system is saved in a file and loaded into our real-time control system package UC ONLINE (see following listing).

A student tutorial, an instructor reference, and sample process diagrams are included. Phone and e-mail technical support is provided. A description of the program features and its use in process control education appeared in Chemical Engineering Education 25, 126 (1991).

Equipment needed:

(1) PC/AT or faster, (2) 640k RAM, (3) EGA or better color display, (4)mouse.

North American academic departmental site license: $500.

A demonstration diskette is available. Address inquiries to:

Prof. Alan Foss
Dept. of Chemical Engineering
University of California
Berkeley, CA 94720

phone (510) 642-4526
FAX (510) 642-4778
INTERNET: online@garnet.berkeley.edu

UC ONLINE - version 2.1: Real-Time Multiloop Control System

Prof. Alan Foss

Almost any imaginable multiloop control system can be placed in operation on laboratory apparatus or simulated processes with this easily learned PC-based computer program. Multiloop feedback, feedforward, and decoupling are easily accomplished. So too are gain schedulers, cascades, overrides, and variable structure systems. System elements at the user's disposal are PID controllers (both velocity and position algorithms), summers, multipliers, dividers, square roots, high- and low-selects, delays, lead-lags, ramps, and sinusoids. All may be speedily incorporated into a full control system through use of our interactive graphics program UC SIGNAL (see preceding listing).

Process simulations and custom modules can be written in Microsoft (tm) Fortran and/or C and linked with the program object modules. A distillation column simulation is available as a separate license.

New features in this version include a screen displaying controller variables and status in a graphical format. One can now bound the rate of change of the output of a controller. Panel displays of system element parameters have been enhanced. Sinusoidal, ramp, and dead-time variables have been added. Controllers now incorporate an audible alarm feature. Datalogging to disk file at user selected intervals has been added. Simulations can now be run at accelerated rates for rapid evaluation of control system performance.

A student tutorial, a user's guide, and an instructor's reference are included. We provide technical support for this product by telephone and/or by electronic mail.

This and earlier versions have been distributed to some 45 institutions worldwide.

Equipment needed:

same as for UC SIGNAL (see preceding listing) except no mouse is required.

North American academic departmental site license: $800.

A demonstration diskette detailing the major features is available.

Address inquiries to:

Prof. Alan Foss
Dept. of Chemical Engineering
University of California
Berkeley, CA 94720

phone (510) 642-4526
fax (510) 642-4778
INTERNET: online@garnet.berkeley.edu
BITNET/EARN:NJE/RSCS:ONLINE at
UCBGARNE.BITNET
UUCP: ucbvax!garnet.berkeley. edu!online

WILSON - A non-ideal vapour-liquid equilibrium tool

by Dr. R.E. Hayes
University of Alberta

WILSON is a software package which performs non-ideal vapour liquid equilibrium calculations and plots phase diagrams. Operations include bubble point, dew point and flash calculations. Plotting options include X vs. Y at constant temperature or pressure with azeotrope prediction, and X and Y vs. pressure or temperature. The program uses the Wilson model for the liquid phase and the virial equation of state for the vapour. The data base provided contains 33 pure components and may be easily expanded by the user. The program is menu driven and has online help available.

This package runs on an IBM PC or compatible equipped with CGA or EGA graphics. WILSON has been used for three years in Chemical Engineering Thermodynamics courses at the University of Alberta.

More information my be obtained from:

Dr. R.E. Hayes
Dept. of Chemical Engineering
University of Alberta
Edmonton, Alberta
T6G 2G6

INTERNET: userhaye@mts.ucs.ualberta.ca
FAX: (403) 492 2881

The following programs have been listed in prior editions of the CACHE News.

1. Vapor compression refrigeration cycle, No. 24 and 25 Stanley Sandler, University of Delaware
2. Compression of an ideal gas, No. 24 and 25, Stanley Sandler, University of Delaware
3. Computer Aided Analysis for Process Systems, No.24 and 25, Ted Cadman, University of Maryland
4. Discounted Cash Flow Analysis (and Present Worth), No. 24 and 25, Bruce A. Finlayson, University of Washington
5. Short-cut Distillation and Flash Calculations, No. 24 and 25, Bruce A. Finlayson, University of Washington
6. Convective Diffusion Equation (CDEQN), No. 25 and 26, Bruce A. Finlayson, University of Washington
7. Engineering Plot (ENGNPLOT), No. 25 and 26, Bruce A. Finlayson, University of Washington
8. Educational Software for Teaching Process Dynamics and Control, No. 26 and 27, Patrick Richard and Jules Thibault, Laval University
9. MIDAS - Microcomputer Integrated Distillation Sequences, No. 26 and 27, Andrew Hrymak, McMaster University
10. A Rigorous Multicomponent Multistage Steady-State Distillation Rating Program, No. 27 and 28, E.C. Roche, Jr., New Jersey Institute of Technology
11. RESIM. A Reactor Design Teaching Tool, No. 27 and 28, B.W. Wojciechowski, Queen's University
12. Real-time Multiloop Computer Control Program, UC ONLINE , No. 27 and 28, by Alan Foss, University of California at Berkeley
13. Real-time Dynamic Distillation Simulation and Relative Gain Program , No. 27 and 28, by Alan Foss , University of California, Berkeley
14. The Kinetics and Selectivity of Consecutive Reactions, No. 29 and 30, by Alvin H. Weiss and Reynold Dodson, Worcester Polytechnic Institute.
15. Equations of State, No. 30 and 31, by Kenneth R. Jolls, Iowa State University.
16. Thermal Design of Shell and Tube Heat Exchangers, No. 31 and 32, by Nurcan Bac and Ilker Ozal, Worcester Polytechnic.
17. Optimum Series Bioreactor Design, No. 31 and 32, by Gordon Hill, University of Saskatchewan.
18. REACT! A Chemical Equilibrium Calculator, No. 32 and 33, by James A. O'Brien, Yale University.
19. BioDesigner, No. 33 and 34, by Demetri Petrides, New Jersey Institute of Technology.

CONFERENCE ANNOUNCEMENT

Foundations of Computer Aided Process Operations

July 18 - 23, 1993
Mount Crested Butte, Colorado

About the FOCAPO II Conference

Process design and process control are well established parts of chemical engineering as taught and practiced at universities and in industry. Such is not the case for process operations. However, market pressures are now compelling process operators to be much more responsive to customer requirements, while economic constraints demand that all advances in overall understanding, system integration and computing capability are called upon to achieve this responsiveness most effectively.

The conference is designed to fill a need not met by other technical conferences and publications. The conference focuses on the need to establish a new discipline of process operations within chemical engineering, integrating technical and commercial considerations and to create new channels of communication and interaction between industry and university on this theme. In depth discussions between university researchers and industrial practitioners offer many opportunities to explore ways to close the gap between theory and practice. Faculty members will be exposed to the stimulus and challenge of operational problems in their wider context, and professionals from industry and government will be sensitized to the potential for fruitful collaboration with universities in research and teaching. Both groups will see ways to enhance the effectiveness of operations in their environment.

Objectives of the Conference

The conference will focus on computational and computer related involvement in plant operations in the process industries. The specific objectives of the conference are:

1. To provide the participants with an appreciation of the state of process operations in several of the process industries, and to obtain from industry a list of future needs and challenges for the research community.

2. To present an overview of the state of the art in theory and practice in a way that is understandable to non-specialists and industrial practitioners.

3. To provide a forum for in depth discussion between university researchers and industrial practitioners on the practical challenges in this field and the extent to which current research directions are satisfying perceived needs.

4. To allow an industrial practitioner to have a better understanding of the new tools available from the research community in order to simulate wider implementation that can be of economic value.

5. To simulate the research community to focus research directions via a better understanding of perceived needs and challenges from the process industries.

The Conference Plan

Location: The conference will be held at the Crested Butte Resort in Mount Crested Butte, Colorado. In the middle of the Gunnison National Forest, the location offers a number of activities such as rafting, ballooning, golf, and tennis. In town, a free shuttle ride away, is the Crested Butte National Historic District with quaint shops, art festivals, concerts, and plays. The hotel is located 210 miles southwest of Denver, and approximately 28 miles from the Gunnison County Airport.

Conference Dates: July 18-23, 1993

Conference Chairmen: Professor David W. T. Rippin
Swiss Federal Institute of Technology (ETH)
Zurich, Switzerland

Dr. John C. Hale
E. I. Du Pont De Nemours & Co.
Newark, DE 19714-6090

Schedule: Morning and evening paper presentations (2 or 3) with discussion. Afternoons available for informal meetings, demonstrations, and special presentations.

Afternoons are traditionally used for informal discussions and personal recreation. Some additional feature activities will be available to expand and enhance the conference: software demonstrations, poster sessions and discussion and formulation of challenge problems typifying important issues in process operations. Offers to contribute to any of these activities may be sent in the form of a 1-2 page abstract to CACHE office (or if you prefer to John Hale at DuPont) not later than January 15, 1993.

Duration: One week of a combination of formal technical sessions and informal discussions, panels, demonstrations, etc.

Size: Limited to 125-150 participants. Experience has shown this is the maximum that can form a cohesive body with the high degree of interaction that is necessary to reach the conference goals.

Diversity: Participants are selected from applicants in order to create diversity in employment (academic, industrial, government), residence (the majority of participants will be US citizens but an international cross section is essential both from Europe and Asia/Pacific), and experience (a range from graduate student to world class experts).

Accommodations and Meals

Arrangements have been made for special room rates at approximately $77 per night for a room with two beds. A conference meal package is planned which includes 3 meals a day and all social functions.

FOCAPO II Program

Sunday, July 18 (PM)

Keynote Talk: Professor Donald Frey
Northwestern University
" Non Steady States - A New Management Paradigm"

Session 1: PROCESS MONITORING ACQUISITION, ORGANIZATION, STORAGE, AND RETRIEVAL FOR REAL TIME APPLICATIONS

Monday, July 19 (AM)

Chair: R.S.H. Mah, Northwestern University

"Data Treatment and Applications"
P. Kennedy, Oil Systems Inc.

"Model Based Monitoring"
R.S.H. Mah, Northwestern University
and M. Kramer, MIT

Commentator: D. Rollins, Iowa State University

Session 2: QUALITY MANAGEMENT

Monday, July 19 (PM)

Chair: E. D. Gilles, University of Stuttgart, Germany

"Design and Control for Quality Improvement in Process Operations"
T. Harris, Queens University, Canada

"Total Quality Management"

Session 3: SAFETY AND ENVIRONMENT

Tuesday, July 20 (AM)

Chair: M. Preston, I.C.I., United Kingdom

"Living with Human Errors on Computer Controlled Plants"
T. Kletz, United Kingdom

"Incorporating Environmental Objectives in Process Design and Operation"
G. McRae, MIT

Session 4: FACILITIES AND PRACTICES TO ENSURE PRODUCT AVAILABILITY

Tuesday, July 20 (PM)

Chair: C.F.H. van Rijn, Shell, Netherlands
Co-Chair: E. O'Shima, Japan

"Total Productive Management in the Refinery of the 21st Century"
(Speaker from Idemitsu Kosan, Japan)

"Managing Reliability and Maintenance in the Process Industry"
J. Grievink, K. Smith, Technical University, Delft
R. Dekkar, Erasmus University, Rotterdam, Netherlands

Commentator: H. Finley, Howard Finley Corp., Houston

Session 5: FLEXIBILITY AND INTEGRATION

Wednesday, July 21 (AM)

Chair: G.V. Reklaitis, Purdue University, USA
Co-Chair: T. Umeda, Sukuba University, Japan

"Outlook for CIM in the Japanese Process Industry"
M. Madono Tonen Systems, and
T. Umeda, Sukuba University, Japan

"Integration of Designs, Scheduling and Control"
S. Macchietto, Imperial College, United Kingdom
Speaker from Shell, Amsterdam, Netherlands

"Integration of Monitoring, Diagnosis and Unit Control"
V. Venkatsubramanian, Purdue University, and
G. Stanley, Gensim

Commentator: V. Mahalec, Aspen Tech

Session 6: Scheduling

Wednesday, July 21 (PM)

Chair: I. Grossmann, Carnegie Mellon University

"An Integrated Approach to Planning and Scheduling"
T.E. Baker, Chesapeake Decision Sciences

"A General Framework for Optimal Process Planning and Scheduling"
C.C. Pantelides, Imperial College, United Kingdom

"Learning to Solve Scheduling Problems - the Role of Rigorous Knowledge Acquisition Framework"
J.F. Pekny, Purdue University

Session 7: PLANT WIDE MANAGEMENT AND CONTROL

Thursday, July 22 (AM)

Chair: I. Rinard, City College of New York

Case Study Presentation
G. Bryant, Imperial College, UK

Session 8: MAKING IT WORK - EXAMPLES OF PROFITABLE APPLICATIONS

Friday, July 23 (AM)

Chair: G. Blau, Dow Elanco

"Achieving the Optimum of a Multiproduct Chemical Plant"
T. Helling, R. D'Sousa, P. Grover, Dow

"A Modular System for Scheduling Chemical Plant Production"
D. L. Miller, H. Singh, K. A. Rogers, DuPont
J.F. Pekny, Purdue University

"A Probability Modeling Methodology for Improving Process Operations"
S. E. Keeler and G. Blau, Dow Elanco

APPLICATION FORM FOR FOCAPO II CONFERENCE

In order to limit the conference size to preserve an atmosphere for creative discussion, attendance at the FOCAPO'93 Conference will be limited and is by invitation following receipt of this application form. You will be notified whether you will be able to attend the conference. The conference fee of $595 will cover registration and a copy of the proceedings. Please complete and send this application by November 15, 1992 to:

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

Name: _____

Title: _____

Affiliation: _____

Mailing Address:

_____

_____

_____

Telephone: _____

Conference Sessions of Main Interest:

_____

_____

Main Area of Research Interest:

_____

_____

Announcements

MicroMENTOR - A Package for Network Management of Instructional Sofware

By Brice Carnahan, University of Michigan

MicroMENTOR consists of three functionally different software suites: (1) System management software; (2) Module (lesson) authoring software; and (3) Instructional modules prepared with the autthoring software.

The System software supports networked management and delivery of almost any educational resource on IBM PC and compatible computers operating under DOS or OS/2. Processed materials may consist of individual DOS line commands, executable and batch files, and educational "modules" (lessons) for computer-assisted instruction (CAI). All files created as a result of user action are maintained in protected MicroMENTOR user directories on the network server(s). MicroMENTOR Controls access to all system resources (by both individual user account/password and priority access level) and automatically compiles statistics on resource use by individual students and groups of students (e.g., a class or department).

Instructional modules can be prepared using a IBM-compatible CAI packatge such as Unison and Quest. In addition, the MicroMENTOR authoring software can be used to prepare MicroMENTOR instructional modules containing submodules whose presentation is menu driven. The student can access (1) tutorials, "lectures/recitations" that allow for student interaction through different logical pathways of almost any complexity; (2) examinations or quizzes, in which all of a student's answers may be saved to server files and later retrieved by an instructor (numerical, multiple choice, true/false, and simple textual - but not essay - responses may also be graded automatically); and (3) application programs, which may demonstrate any of the module topics (for example, through simulations).

Several MicroMENTOR modules for use in chemical engineering courses and/or as generic tools for numerical mathematicsand functional optimization are also available:

1. FLOWSIM	a. Interactive process flowsheet generator b. Steady-state process simulator (materialbalances only)
2. MCCCABE	Mccabe-Thiele binary distillation
3. PONCHON	Ponchon-Savarit binary distillation
4. ROMBERG	Romberg integration
5. LINEQ	Linerar equations (LU decomposition)
6. NEWRAP	Simultaneous nonlinear design equations (more variables than equation) by (damped) Newton-Raphson/ Marquardt
7. RK4	Simultaneous nonlinerar ordinary differen tial equations (4th-orderRunge-Kutta)
8. LINPRO	Linear programming
9. UNLP1	Unconstrained nonlinear programming (Davidon- Fletcher/Powell/Broyden)

For information about availability and cost of the MicroMENTOR software, write to

Prof. Brice Carnahan
Chemical Engineering Dept.
University of Michigan
Ann Arbor, MI 48109.

AspenTech Makes Available University Licenses for ADVENT Pinch Technology Software

By Su Ahmad, Aspen Technology Inc.

ADVENT is a state-of-the-art software tool for applying process integration using Pinch Technology. It is used by several large engineering and operating companies around the world to design for savings in energy and capital. It is also used by some universities in their teaching and research of subjects in process synthesis, process design, heat integration, retrofit methods, etc.

ADVENT is a highly graphical and highly interactive tool. It contains all of the features necessary for applying Pinch Technology, including:

- Targeting (energy and capital), Composite diagrams, Multiple utilities
- Heat and Power Systems (Furnace, Refrigeration, Turbines)
- Heat Exchanger Network Design
- Heat Exchanger Network Simulation and Optimization

ADVENT also has an interface to the ASPEN PLUS process simulator. This is powerful for analyzing process modifications and obtaining stream information including physical properties.

A major new release of ADVENT, Version 4.1, was issued by AspenTech in April this year and incorporates many of the recent advances in Pinch Technology. New features include energy diagrams, shaftwork targets, multiple utilities optimization (with heat and power systems), and multistream heat exchangers. In addition, data management and program navigation are greatly simplified, and on-line help is substantially enhanced.

ADVENT runs under Unix with X-Windows and Motif, and is currently available on either 386/486 PC or DEC-Stations. A version for the Sun 4 sparcstation is planned for late 1992.

AspenTech is currently promoting the ADVENT software to the increasing number of universities which conduct teaching and research of process integration or process synthesis. Only a nominal fee is requested by AspenTech for the University License of ADVENT, and this is intended to cover the cost of media, distribution and some support.

AspenTech recognizes that Pinch Technology is becoming a standard part of design teaching and research. The purpose of our University Program is to increase the classroom experience with using such methods in order to improve productivity, and to encourage R&D projects which emphasize computer-aided process design work.

For more information on obtaining an ADVENT University License, please contact:

Susan Palumbo
Aspen Technology, Inc.
251 Vassar Street
Cambridge, MA 02139

Phone (617) 497-9010
Fax (617) 497-7806

ORDER FORM

CACHE Process Design Case Study Vol. 6
Chemical Engineering Optimization Models with GAMS

The objective of this case study is to provide a set of chemical engineering problems to supplement optimization courses at both the undergraduate and graduate level. This case study should also be useful in othercourses and to practicing engineers to learn about GAMS and its applications.

Gams is an algebraic modeling system in which the user need not be concerned with details of providing the interfaces with various optimization codes. Instead, the GAMS environment allows the user to *concentrate on the modeling of problems*, which ultimately is the main skill that is required for the successful application of optimization in practice. This case study covers applications at various levels of complexity in the following areas: (a) Planning and scheduling of batch and continuous processes, (b) Chemical and phase equilibrium, (c) Design of heat exchanger networks, distillation columns and batch processes, (d) Synthesis of reaction paths, heat exchanger networks and distillation sequences, (e) Optimization of dynamic and distributed parameter models. These problems are modeled as linear, nonlinear and mixed-integer optimization problems.

This case study describes in detail the formulation and solution of a total of 22 optimization problems that cover the different areas cited above. Exercises are also given for each problem. In addition, the case study includes:

a) Special student version of GAMS for IBM-PC and compatibles in 3.5" diskettes. The MINOS, ZOOM and DICOPT++ codes are included in this GAMS version which can handle problems with up to 1000 nonzero elements in the Jacobian matrix.
b) GAMS input files for all the problems; these are extensively documented.
c) GAMS User's Guide.

This case study has been prepared by faculty and students from Carnegie Mellon University, Northwestern University and Princeton University under the coordination of Ignacio E. Grossmann. GAMS Development Corporation, the Licensing Technology Office at Stanford University, and XMP Optimization Software have donated the computer software for this case study.

CACHE PROCESS DESIGN CASE STUDY VOLUME 6
"Chemical Engineering Optimization Models with GAMS"

# of copies:		Total
_____	$55 for CACHE-supporting department	_____
_____	$80 for non-supporting departments	_____
	TOTAL	_____

Name: _____

Address: _____

_____

_____

Make check payable to CACHE Corporation.

Please mail order form to:

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

POLYMATH Order Form

If you decide to obtain POLYMATH for testing (see form below), please be aware of the following:

1. **You may reproduce the program as many times as you like for students and other faculty.**
2. **Your department chairman will be informed of the testing.**
3. **If you decide to use POLYMATH in your department after 3 months, your department will be billed for $125.00, and $75.00 for each successive year thereafter. This fee covers any updates or new versions.**
4. **If you decide not to use POLYMATH after 3 months, you must return (or certify you have erased) all copies made.**
6. **Educational supporting material will be available from CACHE later in the year at $50.00 per copy.**

Please send me a copy of POLYMATH for the IBM/PC. I have read and understood the conditions described above.

Date: _____

Requested Disk:

[ ] 5 1/4" Double Density

[ ] 5 1/4" High Density

[ ] 3 1/2" High Density

Name _____

Address _____

_____

_____

Machine _____

Make check payable to CACHE Corporation and send to:

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

CACHE
Model Predictive Control Toolbox
(CACHE-Tools)

MATLAB Functions for the Analysis and Design of Model Predictive Control Systems

Model Predictive Control Toolbox
Site-License

[ ] $ 160 for CACHE-supporting departments

[ ] $ 250 for non-supporting departments

[ ] $ 1000 for non-supporting companies

[ ] 3.5" PC-disk [ ] 4.25" PC-disk [ ] 3.5" Macintosh-disk

Name: _____

Address: _____

_____

_____

_____

_____

Make check payable to CACHE Corporation and send to:

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

FLOWTRAN TAPE ORDER FORM

_____ I am interested in preparing a FLOWTRAN tape.

_____ I am interested in obtaining a FLOWTRAN tape.

If you have checked either of the above, please complete the following information. If you have two computers you want to consider, duplicate this form and 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: _____
5. No. of tracks: _____
6. Drive speed in bits/inch: _____

Send form to:
Professor J. D. Seader/CACHE
3290 MEB
University of Utah
Salt Lake City, UT 84112

Note:
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. The charge to CACHE-supporting departments is $175.

FLOWTRAN BOOKS ORDER FORM

Please send me:
Flowtran Simulation - An Introduction, 3rd edition; Pauls.

No. of copies: _____ at $16.95/copy

Name: _____
Address: _____
_____
_____
_____

Send form to: ULRICH'S Bookstore
ATTN: Heather Senior
549 E. University Avenue
Ann Arbor, MI 48109

Add $1.50 per copy for mailing and handling in the U.S.
A check must accompany all orders by individuals. Also available in quantity at regular quantity discounts to established book retailers. Make checks payable to Ulrich's Bookstore.

STANDARD ORDER FORM

Description of Item	Quantity	Unit Price		Total
		Supporting	Non-supporting	
AI Monograph - Volume 1		$15	$15	
AI Monograph - Volume 2		$15	$15	
AI Monograph - Volume 3		$15	$15	
Set (1,2, and 3)		$15	$15	
AI Case Study - Volume 1		$10	$17	
AI Case Study - Volume 2		$10	$17	
AI Case Study - Volume 3		$10	$17	
Set (1,2, and 3)		$10	$35	
GPSS		$15	$15	
PIP		$50	$75	
Process Design Case Study Volume 4		$15	$35	
Process Design Case Study Volume 5		$20	$40	
Process Design Case Study Volume 6		$55	$80	

Name: _____

Address: _____

_____

_____

_____

Please make checks payable to CACHE Corporation
in U.S. funds and drawn on a U. S. Bank and return to:

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

For a complete listing of CACHE products, send in for a CACHE catalog.

INDUSTRIAL CONTRIBUTORS TO CACHE

The following companies have recently contributed financial support to specific CACHE activities:

DuPont Committee on Educational Aid

Tektronix

Xerox Foundation

List of Chemical Engineering Departments Supporting CACHE

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

Auburn University
Tuskegee University
University of Alabama, Tuscaloosa
University of South Alabama
Arizona State University
University of Arizona
University of Arkansas
University of California, Berkeley
University of California, Davis
University of California, Los Angeles
University of California, Santa Barbara
California Institute of Technology
California State Polytechnic University, Pomona
University of Southern California
University of Colorado
Colorado School of Mines
Colorado State University
University of Connecticut
University of Delaware
Howard University
University of South Florida
Georgia Institute of Technology
University of Idaho
University of Illinois, Chicago
University of Illinois, Urbana
Illinois Institute of Technology
Northwestern University
Purdue University
University of Notre Dame
Rose-Hulman Institute of Technology
Tri-State University
University of Iowa
Iowa State University of Sci. & Tech.
University of Kansas
Kansas State University
University of Kentucky
University of Louisville
Louisiana Technical University
Louisiana State University
Tulane University
University of Southwestern Louisiana
University of Maine
Johns Hopkins University
University of Maryland
Massachusetts Institute of Technology
University of Lowell
University of Massachusetts, Amherst
Northeastern University
Tufts University
Worcester Polytechnic Institute
University of Michigan
Michigan State University
Michigan Technological University
Wayne State University
University of Minnesota, Duluth
University of Minnesota, Minneapolis
University of Mississippi
University of Missouri, Columbia
University of Missouri, Rolla
Washington University
University of Nebraska, Lincoln
University of New Hampshire
Dartmouth College
New Jersey Institute of Technology
Princeton University
Stevens Institute of Technology
University of New Mexico
City College of the City University of New York
Clarkson University
Cornell University
Manhattan College
Polytechnic University
Rensselaer Polytechnic Institute
University of Rochester
State U. of New York at Buffalo
Syracuse University
N. Carolina State University, Raleigh
N. Carolina A&T State University
University of North Dakota
University of Akron
Case Western Reserve University
University of Cincinnati
Cleveland State University
University of Dayton
Ohio State University
Ohio University
University of Toledo
Youngstown State University
University of Oklahoma
University of Tusla
Oklahoma State University
Oregon State University
Bucknell University
Carnegie Mellon University
Lafayette College
Lehigh University
University of Pennsylvania
Pennsylvania State University
University of Pittsburgh
Villanoava University
Widener University
University of Puerto Rico
University of Rhode Island
Clemenson University
S. Dakota School of Mines & Tech.
University of Tennessee, Knoxville
Vanderbilt University
Lamar University
University of Texas at Austin
University of Houston
Rice University
Texas A&M University
University of Utah
Brigham Young University
University of Virginia
Hampton University, Virginia
Washington State University
University of Washington
University of West Virginia College of Graduate Studies
W. Virginia Institite of Technology
W. Virginia University
University of Wisconsin
University of Wyoming
University of Adelaide, South Australia
University of New South Wales, Australia
University of Sidney, Australia
University of Alberta
Ecole Polytechnique—U. of Montreal
Lakehead University
Laval University
McGill University
McMaster University
Queen's University
Royal Military College of Canada
Technical University of Nova Scotia
University of British Columbia
University of Calgary
University of New Brunswick
University of Ottawa
University of Saskatchewan
University of Sherbrooke
University of Toronto
University of Waterloo
University of Concepcion, Chile
University of Bath, England
University of Oulu, Finland
University of Stuttgart, Germany
Imperial College, Great Britain
Indian Institute of Technology
Cork Regional Tech. College, Ireland
University College, Dublin, Ireland
Technion-Isreal Inst. Tech. - Isreal
Kyoto University, Japan
KAIST, Korea
Pohang Institute of Science & Technolgy, Korea
Norwegian Institute of Technology
King Abdulaziz U., Saudi Arabia
University of Cape Town, So. Africa
Escuela de Ingenieros, Spain
ETH Zentrum, Switzerland
Institute D'Automatique, EPFL, Switzerland
University of Maribor, Slovenia
Chulalongkorn University, Thailand
Middle East Tech. University, Turkey

Topics in this issue of the CACHE Newsletter:

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

Nonprofit Organization
U.S. Postage Paid
Austin, TX
Permit No. 699