CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 31 Fall 1990

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:

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

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! N O T I C E !

CONCERNING ELECTRONIC MAIL ADDRESSES OF CHEMICAL ENGINEERING FACULTY

A list of electronic mail addresses for chemical engineering faculty has been compiled and may now be accessed by sending electronic mail to:

chelib@emx.utexas.edu

This list will allow you to obtain up-to-date e-mail addresses of chemical engineering faculty via electronic mail. It works by replying automatically to your request.

To search for someone in the faculty address list, send the one line:

Who is Joan Doe

to chelib@emx.utexas.edu. You will receive a reply by return mail which displays all entries containing the string "Joan Doe". The search is not case sensitive, and no spelling correction is attempted. You may include several requests in a single piece of mail, but put each on a separate line.

Send the requests to chelib@emx.utexas.edu even though replies appear to be coming from chelibd@emx.utexas.edu. You will be talking to a program, so do not expect it to understand much English.

To receive the entire list of e-mail addresses of Chemical Engineering faculty, send the message:

Send addresses from faculty

Please send any corrections and additions to:

chelib-request@emx.utexas.edu

The list will be updated as time permits.

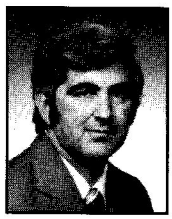
In the future, other interesting things may be available from chelib. To receive an index of currently available items, send the message:

Send index

The POLYMATH Numerical Computation Package

By Michael Cutlip, University of Connecticut
and Mordechai Shacham, Ben Gurion University of the Negev, Israel

Michael B. Cutlip is Professor of Chemical Engineering at the University of Connecticut. He is a B.Ch.E. and M.S. graduate of the Ohio State University and obtained his Ph.D. at the University of Colorado. Most of his academic career has been at the University of Connecticut where he has just completed a nine year term as department head. His research interests encompass transient studies of heterogeneous catalysis and electrochemical engineering of fuel cell systems. He has helped to develop computer-based instructional materials in reaction engineering and has coauthored the POLYMATH package for numerical analysis on a PC. He has been a visiting professor at Michigan and recently at the University of Adelaide in South Australia. He has spent two years at Cambridge University as a senior visiting fellow and will visit Japan this spring as a JSPS fellow. He is a CACHE Trustee and currently serves as secretary.



Mordechai Shacham is currently Professor of Chemical Engineering at the Ben Gurion University of the Negev in Beer Sheva, Israel. He received his BSc and DSc from the Technion, Israel Institute of Technology. He spent a year as a visiting faculty member at the University of Houston in 1974, and two years at the University of Connecticut in 1979-81. Dr. Shacham was the head of the Chemical Engineering Department at the Ben Gurion University from 1985-1989, and he is currently the president of the Israel Institute of Chemical Engineers. His research interests include: applied numerical methods, computer aided instruction, chemical process simulation, design and optimization, and expert systems.

POLYMATH is a software package that we have developed that is useful for a wide variety of numerical computations employed to solve chemical engineering student problems. We have been using this package for about seven years as a computational tool in both graduate and undergraduate courses. The package is now being made available for all the Chemical Engineering Departments via CACHE.

These programs are equation and data oriented in that all the equations can be typed in their regular algebraic form with the user's own notation. The best solution algorithms are automatically determined, and solutions are presented in numerical, tubular, or graphical form. The structure of the programs and typical examples of where they can be used are given in detail in the references by Shacham and Cutlip listed at the end of this article. Our experience has shown that the major benefit of POLYMATH is that it allows solution of realistic problems without requiring excessive student time.

A form to order POLYMATH will be found at the end of this newsletter. The package runs on IBM PC/XT, AT, PS/2 and most compatibles. It requires a color graphics board: CGA, EGA, VGA or Hercules.

The Polymath Software

The POLYMATH package has been designed for general purpose use by faculty and students who can formulate problems in mathematical terms. The programs are extremely easy to use, and all options are menu driven. Equations are entered in standard form with user-defined notation. Results are presented in graphical or tabular form. No computer language is used, and a manual is really not required for normal use. All problems can be stored on disk for future use. A calculator and unit conversion utility are always available.

POLYMATH is very useful as general problem solving software throughout the Chemical Engineering curriculum. POLYMATH improves faculty and student ability to solve more realistic numerical problems which reduces emphasis on the details of the computing. It can also be used to support courses in numerical analysis as details on the numerical methods are

given in help sections of the programs. Typically, POLYMATH is provided in personal computer labs and/or given to individual faculty and students.

There are currently five programs which provide the basic numerical methods:

Curve Fitting Program - The user can input up to 99 data points. Major options for data fitting include polynomials to the 5th degree, cubic spline, and linear interpolation. Fitted curves can be interpolated, differentiated, and integrated. Input data can be transformed. Graphical output of fitted curves is given.

Algebraic Equation Solver - The user can solve up to a combination of 12 simultaneous equations and explicit algebraic expressions. All equations are checked for correct syntax and other errors upon entry. Equations can easily be modified, added or deleted. Multiple roots are given for a single equation. A separate simple linear equation solver handles up to 6 simultaneous equations.

Differential Equation Solver - This program allows the numerical integration of up to twelve nonlinear ordinary differential equations and algebraic expressions. All equations are checked for syntax upon entry. Equations are easily modified. Initial values must be provided. Undefined variables are identified. Integration method and stepsize are automatically selected. Graphical output of problem variables is easily obtained using automatic scaling.

Multiple Regression Program - Up to 100 data points consisting of a dependent variable and a maximum of four independent variables can be handled. A linear regression including an option for zero intercept is performed giving a variance. Graphical output is provided. User defined transformation function can be used to linearize complicated expression for regression.

Matrix Manipulation Program - This POLYMATH program allows the use of spread-sheet type commands to input, store, edit, and evaluate expressions consisting of vectors and matrices. Selected operations range from simple vector operations through matrix multiplication and inversion to Eigenvalue and Eigenvector calculations. Algebraic expresssions entered in standard matrix notation are easily evaluated.

In What Courses is POLYMATH Useful?

Following is a list of problems which have been solved by students, in different ChE courses, using POLYMATH. Once the mathematical representation of the problem has been developed, the solution time is essentially the time required to type in the equations or the numerical data.

For problems which are available in the open literature, the reference is given in parenthesis.

Material and Energy Balance

1. Williams-Otto process (Henley and Rosen (1969), p. 408)
2. Shell and tube heat exchanger (Shacham (1989))
3. Cross current extraction (Chang and Over (1981))
4. Rigorous energy balance on a shell and tube heat exchanger (Carnahan et al. (1969), p. 132)
5. Material balance on a complicated recycle system (Henley and Rosen (1969), pp. 421-424)

Thermodynamics

1. Wilson equation parameters from composition and activity coefficient data (Chang and Over (1981), p. 196)
2. Adiabatic flame temperature in combustion
3. Solution of equations of state for volume or compressibility factor (Beattie-Bridgeman, Carnahan et al (1969), p. 173, Virial, Chang and Over (1981), p. 7, Benedict-Webb-Rubin)
4. Activity coefficient consistency tent (Sandler (1989), p. 397)
5. Integration of heat capacity data to calculate enthalpy

Correlation of properties

1. Vapor pressure using Antoine equation (Myers and Seider (1976), p. 195)
2. Latent heat of vaporization (Myers and Seider (1976), p. 166)
3. Viscosity (Myers and Seider (1976), p. 195)
4. Vapor-liquid equilibrium data

Fluid Flow

1. Flow and pressure drop in pipeline networks (Gerald and Wheatley (1984), p. 170, Carnahan et al. (1969), p. 310, p. 337)
2. Isentropic flow through a converging diverging nozzle (Carnahan et al. (1969), p. 204)
3. Correlation of fluid flow as a function of diameter and slope

4. Dynamic response of a surge tank (Carnahan et al. (1969), p. 421)

Phase equilibrium

1. Azeotropic point calculation
2. Ideal multicomponent mixture: dew point, bubble point and isothermal flash
3. Nonideal vapor-liquid and liquid-liquid equilibrium (Henley and Rosen (1969), pp. 348-353)

Distillation

1. Short-cut distillation (number of trays at infinite reflux, minimum reflux, feed tray location) of a multicomponent mixture.
2. Demonstration of the Wang and Hanke method for binary distillation.

Heat Transfer

1. Heat transfer correlation in a heat exhanger (Carnahan et al. (1969), p. 591)
2. Heat transfer correlation in a fluidized bed reactor (Lapidus, L. (1962), p. 354)

Chemical Reaction Engineering

1. Volume and conversion in consecutive CSTR's (Carnahan et al. (1969), p. 202)
2. Chemical equilibrium (Shacham (1989))
3. Synthesis gas production (Carnahan et al. (1969), p. 321)
4. Complex chemical equilibrium (Shacham 1983)
5. Determination of rate law parameters for catalytic reaction (Fogler (1986), pp. 261-268)
6. Differential method or rate data analysis (Hill (1977), p. 44)
7. Integral method of rate data analysis (Hill (1977), p. 44)
8. Use of conductivity measurements to determine rate constants (Hill (1977), p. 61)
9. Activation energy from rate coefficient data (Smith (1981), p. 48)
10. Rate data analysis using the method of half-lives
11. Method of initial rates
12. Material and energy balance on a nonisothermal CSTR (Luyben (1974), p. 144)
13. Material and energy balance on a tubular reactor (Carnahan (1969), p. 353)
14. Pressure drop and conversion in a packed bed reactor (Fogler (1986), p. 131)
15. Isothermal Semibatch Reactor (Fogler (1986), p. 148)
16. Inert membrane reactor (Fogler, 2nd Ed.)
17. Decay in a straight through reactor (Fogler, 2nd Ed.)
18. Operation of a plug flow reactor with heat exchange (Fogler, 2nd Ed.)
19. Adiabatic batch reactor (Fogler (1986), p. 148)
20. Glucose to ethanol fermentation in a batch reactor (Fogler, 2nd Ed.)
21. Catalyst decay in a CSTR (Fogler (1986), p. 278)

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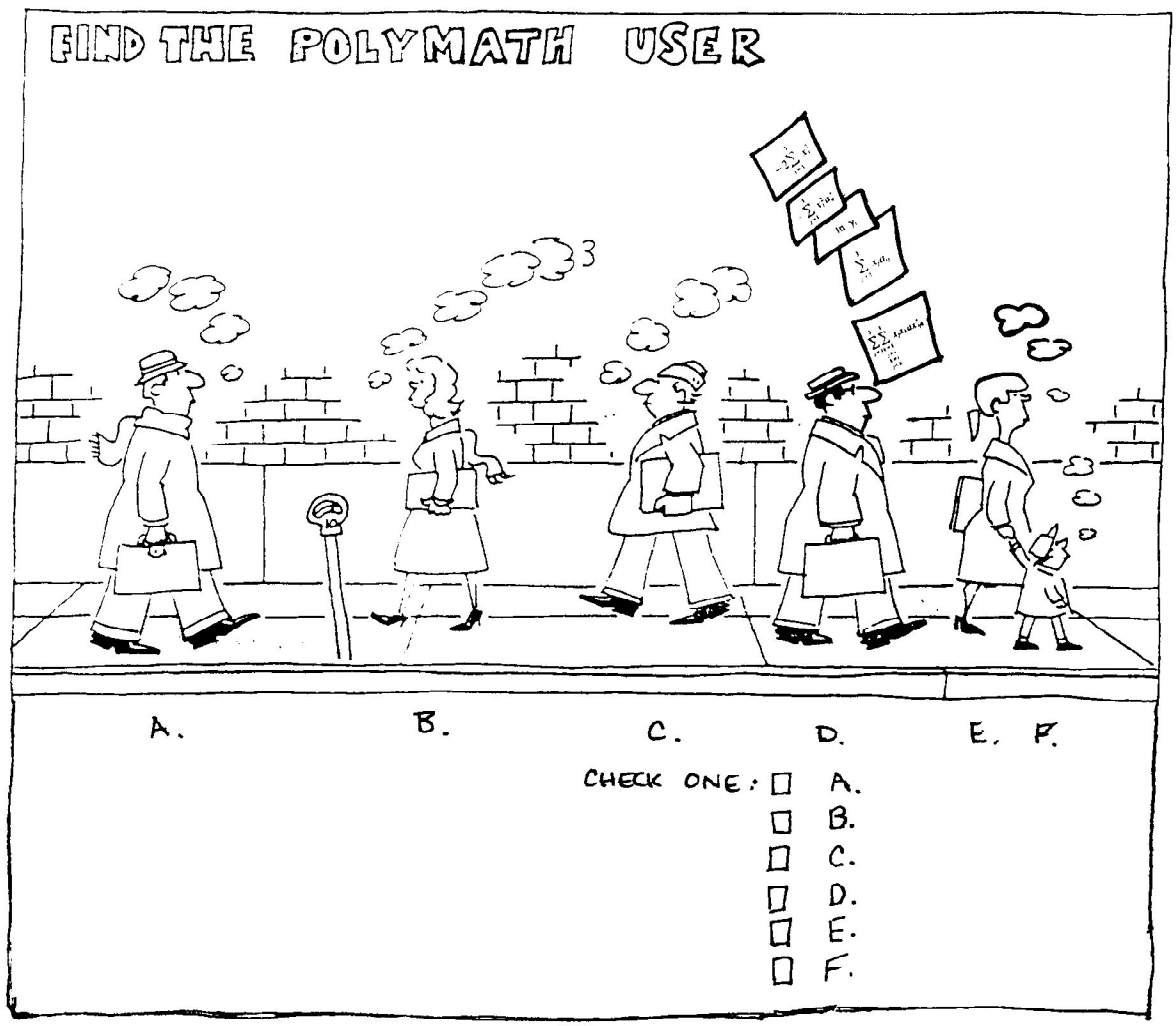

Electronic Technical Publishing (ETP)

Richard S. Mah, Northwestern University, Brice Carnahan, Michigan University and Peter Rony, Virginia Tech

What Is ETP?

Computers have deeply affected the way we function as chemical engineers. One such function which has undergone dramatic changes over a period of less than 10 years is the preparation and dissemination of a technical document. This is a function which touches every chemical engineer at one time or another, as author, reviewer, editor and reader. The technical document concerned could be a manual, a research paper, a thesis, a textbook, and so on. Equations, tables, figures, references and notation are central to these documents. Electronic technical publishing (ETP) is a term we use to describe collectively the software and hardware technology devised to assist this function.

Potentially, ETP can be a great bonus to our profession. Chemical engineering is undergoing rapid change. We are opening up new frontiers. We need to communicate new research findings. We need new textbooks for new courses. But we do not have the large markets of electrical and mechanical engineers. ETP allows us to prepare camera-ready manuscripts which can be quickly and cheaply turned into hard cover textbooks and research monographs. ETP allows rapid and frequent updating of material. Computer simulation and graphics display which could not be disseminated widely and easily before are now suddenly accessible around the globe on desktops. The ramifications of these changes as they affect authors, readers, publishers and our profession are both broad and profound. An *ad hoc* committee was appointed by CACHE to gather information and develop guidelines which may help chemical engineers in their various roles associated with ETP. We choose to report our findings in the format of newsletter articles. This format was chosen for two reasons. First, it shortens the time of preparation and communication. Second, being an open-ended media, it allows the readers to participate in the discussion through letters to the editor.

We focus our report on the preparation and production of documents, and group our discussions around three types of issues: Software, hardware and institutional. The first two issues will be addressed in this article.

Software Issues

Starting Point: Your Requirements

At this point, there is a bewildering range of software and hardware options to choose from. The logical starting point is to define your requirements: the length of your document and its makeup in terms of text, symbols, equations, operators, fonts, tables, figures, format, style, and so on. A 20-page document probably does not need indexing, running heads, and table of contents, all of which are important in a 500-page book. If the material contains a lot of equations, then technical word processing may become more important than document management. If it contains many figures, then the graphics capabilities of the software may assume greater significance. The more thoroughly you can specify your requirements, the more readily you can make the selection of software. What follows is a list of software issues that must be considered.

Text Creation and Editing

Some desktop publishing software (e.g., Ventura) allows text prepared on another word processor (e.g., WordStar, Word Perfect, Microsoft Word) to be imported. Others provide full text preparation facilities. In either case the word processing capabilities should feature *copy*, *cut* and *paste*, *search* and *replace*, and the ability to handle at least two files simultaneously (e.g., through two windows). It should also support *typefaces*

and *fonts* that you want to use (see Appendix for further details). Many ETP software packages (e.g., Lotus MS and Ventura) also provides thesaurus, hyphenation and spelling dictionaries, both standard and customized.

Markup, WYSIWIG and Hybrids

The traditional approach to manuscript preparation is to embed format commands in a document source file. The formatter uses a markup language to transmit the instructions. *Markup languages* (See Glossary for definition) have been developed for tables, equations, pictures, graphs, and so on. T_EX is probably the best known program using this approach. In the Unix environment, troff is widely used.

Learning a markup language requires a significant effort. Markup files are not very readable. A more friendly approach is called *WYSIWYG* ("what you see is what you get"). Editing requests are applied directly to the document image. Text and formatting codes are inserted in a file that is unseen by the author. This approach is widely used in the PC environment (e.g., T^3 software). It does not generally offer the same degree of control over the quality of final document, and is often slower.

Some ETP software adopts a compromise - a hybrid between these two extremes. Lotus Manuscript, for instance, lets you format as you compose. But to see a page layout, the user has to activate a graphics display monitor through a preview mode. The normal display shows only ASCII characters; attributes such as bold, italic, subscript and superscript may be color coded. The display is quite readable and fast. However, one serious drawback is that without using a print formatter/previewer there is no clear indication of page boundaries, which makes it very hard to do page layout in a long document.

Equations and Symbols

There are now more than a dozen technical word processing programs available (see PC Magazine, July 1988, pages 251-328 for a review). However, the issue here is completeness and convenience. For example, does the software allow boldface attributes for Greek, script, parentheses and brackets? If it does not, and you need them, then the software may not be appropriate for you. Another example is matrices. Many packages support matrices, but sometimes you may wish to annotate rows and columns of a matrix. Does the software support such capability? For a short document you may elect to cut-and-paste around the limitations, but for a longer document are you prepared to change your writing style? Sometimes, even when the capability is provided in theory, it may not be convenient to use repeatedly. For example, equations may have to be prepared using different software and transferred and pasted, files may have to be opened and closed each time, or many keystrokes may be required to create a symbol. You may be prepared to do it for a short document, but for a book....?

Tables and Figures

A well-designed table facility can be a most valuable asset in ETP software. A table with flexible bordering options can be used to prepare simple figures. But, of course, it is not a replacement for a general graphics capability. Most packages will allow whitespace (blank space) to be inserted. Some will allow compatible graphics to be imported. But for page layout of a long document, it will save a lot of time to be able to create and size figures within a document. This capability does not currently exist in most software packages.

Document Management

For a long document, you would like to have different page formats for the title page, first page, even page, odd page, and so on; different running heads for even and odd pages, table of contents, footnotes and indexes, which will keep track in spite of document modifications. Some software allows you to create a document in any order you like, and contract and expand the display at different levels at will. A recent supplement to PC Week (August 21, 1989) listed some 17 page-layout software packages, each under $600, that does not even cover any of our favorites.

Platforms

Many of the earlier software - such as RUNOFF, troff, Scribe and T_EX - were available only on workstations or mainframes. Unix is a common platform for many such packages. Some ETP software has been adapted for different platforms and hardware, e.g., MicroTex and PC TeX for IBM PC compatibles, MacTex and $T_EX$tures for the Macintosh. Also, some software has been simplified

and improved (e.g., LATEX). At this time, good ETP software is available under DOS, OS/2, Unix or (Macintosh) Finder. If you are careful, you may even be able to migrate from one hardware platform to another.

Learning Effort

Full-fledged ETP software offers a wide range of commands; learning to use it definitely requires an effort. If it is a well-designed package, you should be able to start out on your own in a few days, but a reasonable expectation is that you will become conversant with it only several hundred pages later. Certain characteristics such as mouse or keyboard orientation may help or hinder your personal adaptation. Some software also offers macro capabilities, but these capabilities are probably not utilized by casual users. In any event, your learning effort should definitely figure in your considerations.

In general, ETP software does not offer online tutorials. But some software vendors provide hotline support, which can be very helpful. Typically, it takes the form of 6- to 12-month support on a 1-800 line, and may be renewed (for a modest price) for further periods on an indefinite basis.

The features of three ETP packages are selected for further comments below.

Lotus Manuscript

Lotus Manuscript is an attractive ETP package that combines technical word processing with document management capabilities. It runs under DOS on an IBM AT or 386 compatible with 640 KB memory and a hard disk. It has an excellent text editor and uses a print formatter/previewer that allows zooming and magnification. Its liberal use of menus and function keys (at 3 different levels) is very economical in keystrokes. It uses markers to introduce special processors and to indicate places in a document where extraneous material belongs. There is a marker for just about anything that is not text: from author, figure, font to orientation, whitespace and worksheet. Particularly noteworthy is the equation marker, which allows the creation and insertion of equations. A most ingenious method is used to entering equations. It is based on the way an equation is read verbally. In other words, so far as equations are concerned, "what you read is what you get" (*WYRIWYG*). For instance, "phi sub [nn] (tau) = 1 over [2 pi] int super infinity sub [- infinity] PHI sub 0 exp(j omega tau) d omega" gives rise to the following equation:

$$\phi_{nn}(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \Phi_0 \exp(j\omega\tau) d\omega$$

Possibly one major weakness of Lotus Manuscript is its graphics. Graphics created using Freelance Plus, Graphwriter, Lotus 1-2-3, and Symphony and other compatible packages can be inserted. But these packages are relatively limited in their capabilities. Lotus Manuscript has excellent format control at the page, block, section, typeface, and attribute levels. At a retail price of $350, this software is a bargain.

Xerox Ventura Publisher

Xerox Ventura Publisher is one of the leading "desktop publishing" software packages available for personal computers. An upgrade - the Professional Extension - has placed this package into the ETP category by providing the following additional features: equations, tables, variable insertion, cross referencing, vertical justification, an expanded 130,000 word hyphenation dictionary, and Expanded Memory Specification (EMS) support. The use of EMS permits a user not only to create larger and more complex documents than is possible with Ventura Publisher alone but also to run disk cache programs to increase processing speed. The equation-writing capability of the Professional Extension is, like Lotus Manuscript, *WYRIWYG*: you write the equation in text form, and the software translates it into a complex mathematical or scientific equation. Among numerous strengths of Ventura Publisher, three - file import capability, tags and style, and frames - deserve special mention.

Ventura allows more than 25 different file types to be imported directly. These include text, line art and image files.

A user develops a "style" in which each different type of paragraph (which could be a single word) has a separate "tag" that characterizes the font, spacing, and other characteristics of the text of equation. A group of related tags collectively comprise a single style; pre-existing style templates are commercially available.

Each page can be subdivided into one or more frames of different sizes and uses. Text that spills over a single frame can be easily continued on subsequent pages. The creation of a textbook typically involves fifty to one hundred separate text, line art, and image files that are melded together by Ventura Publisher.

TEX

TEX, developed by Donald Knuth of Stanford University, is probably the most widely used of the markup languages. It is a *typesetting* rather than a word processing language with the mission of producing "beautiful" technical documents. It is copyrighted, and has just one set of marks and syntactical rules, regardless of the hardware and operating system used.

A TEX source document can be prepared using *any* ASCII editor on *any* computer, and is completely transportable from one platform to another. TEX compilers are widely available on vertually every computer from mainframe to PC.

Every TEX compiler produces an output document file that is identical and independent of the eventual output device, be it a desktop laser printer or a 2400 dpi (dots per inch) Mergenthaler typesetter. Device-dependent programs (drivers) for transforming the output file into typeset or printed output are available for almost all standard output devices.

TEX is the official document-preparation language for several important technical journals, e.g., publications of the Americal Mathematical Society.

TEX incorporates many system-defined macros, and allows a knowledgeable user to create other macros that permit a document to be formatted in virtually any style. Its compilers have powerful built-in typesetting heuristics for automatic hyphenation, justification, kerning, and equation and table formatting. In addition, TEX incorporates a flexible space allocation feature called "glue" that allows it to reposition material on each page automatically to produce pages that "look good". It also allows manual intervention, if the results are less than totally satisfactory.

On the other hand, automatic spelling checking and index generation are not available as standard features in most TEX implementations. TEX has virtually none of the *WYSIWYG* features that most of us like in ETP software. For example, consider the following typeset equation:

$$\eta = 26.69\frac{(MT)^{1/2}}{\sigma^2\Omega_v} \qquad (1)$$

The original TEX source code for generating this equation would appear as follows:

```
$$\eta =26.69{(MT)^{1/2}\over\sigma^2\Omega-v
\eqno(1)$$
```

This input code is rather archaic (though fairly obvious). As the complexity of equations and tables increases, the TEX advantage becomes more obvious.

Typically, it takes several days to become productive with the language, and perhaps a month of full-time use to become truly fluent and reasonably expert. In summary, TEX is a powerful tool for preparing good-looking technical documents. The language is complex, a bit arcane, and probably not worth the steep learning curve if one plans to create only short, mostly textual, documents. But if one frequently prepares highly technical and lengthy documents containing tables and equations, one should consider TEX as a possible authoring tool.

Hardware Issues

Monitors

A monitor is a two-dimensional, cathode-ray tube (CRT) screen that is traversed by a beam of electrons both vertically and horizontally. The technique is called raster scanning. The horizontal trace, from left to right as you view the screen, is done at the highest possible frequency, which dictates the quality of the screen images that can be displayed. In contrast, the vertical frequency is done at the lowest possible frequency consistent with the absence of annoying flicker on the display. A typical monitor contains 25 rows of 80 characters; each character

consists of a 7 by 7 dot matrix framed within a 8 by 8 character box that has a total of 64 pixels. The maximum number of pixels on a horizontal and vertical line, called the resolution, is derived from the bandwidth, horizontal scan frequency, and vertical scan frequency characteristics.

Pioneered by NEC in Japan with its MultiSync family of monitors, multifrequency scanning of horizontal lines has become widespread in the last several years. Instead of a monitor being restricted to the TV standard horizontal and vertical scanning rates of 15.750 kHz and 60 Hz, respectively, the MultiSync monitor can accept a variety of scanning rates, and thus can track technological advances in video boards (CGA, EGA, MCGA, VGA, for example) without monitor replacement.

In a bit-mapped video display, there is a bit stored in memory for every bit required by the monitor. For example, an IBM CGA display has 640 x 200 = 128,000 pixels in its high-resolution mode. If 160 x 100 pixel resolution is acceptable, 4 bits (corresponding to 16 different colors) can be employed to store color information. Clearly, there is a tradeoff between number of colors and resolution on the RGB color monitor. In an alphanumeric video display, there is one byte of memory storage for every character required by the monitor. For example, a typical monochrome monitor displays 25 lines of 80 characters each, or a total of 2000 characters (2000 bytes). Graphics display standards are known by the acronyms MDA, CGA, EGA, VGA, MCGA, EVGA and XGA. A monitor that receives only digital signals provides only a discrete number of different colors. For the VGA standard, 6 bits are stored for each of the three primary colors red, green, and blue. A total of 18 bits means 262,144 different colors. The Macintosh II stores 8 bits per color, corresponding to a total of 24 bits and 16,777,216 different colors.

Page Printers

Of the seven basic types of hardcopy devices - dot matrix, letter quality (character), plotter, ink-jet, thermal, laser, and phototypesetter - only the last two or three types provide qualities sufficient for ETP applications. A "printer" in the context of this discussion means a page-printer of the laser type (or one or two technological equivalents) that provides printing quality of at least 300 dpi and a printing speed of at least six pages per minute.

A critical issue in selecting a laser printer is not the manufacturer, the cost, the speed, or the printing resolution, but rather the electronic output file format that the printer accepts and converts into printed pages. This is a critical issue, because a careful decision concerning output file format may well provide access not only to a laser printer (300 dpi resolution), but also to a phototypesetter such as a Linotype machine (1200 dpi resolution). In other words, if you are careful you may be able to print copies of your book or manuscript for limited initial distribution yet retain the possibility of higher quality printing should your work prove to be popular.

As explained in a printer manual, "control codes and escape sequences are special messages that your computer sends to the printer. These messages change the way the printer is currently printing and give you control over the appearance of your output. The printer receives each control code as a single character of information. Escape sequences are two or more characters of information. Like control codes, they let you change the way the printer is currently printing..." The unfortunate aspect of printer technology is that output file formats (including control codes and escape sequences) are not standard among all printers. De facto standards have been and continue to be created for the most popular printers, examples of which include:

Diablo 630 format	letter quality printer
Epson FX-80 format	dot matrix printer
PostScript format	laser printer, typesetter
IBM Proprinter format	dot-matrix printer
Hewlett Packard LaserJet Plus format	laser printer
Hewlett Packard Graphics Language (HPGL) format	plotter

Electronic technical publishing software, for example, Lotus Manuscript, Microsoft Word for Windows, Pagemaker, and Ventura Publisher Professional, must provide printer output files that contain control codes and escape sequences for one or more designated printers. There is a clear distinction between the output file formats for the two major contenders in the personal computer market: Apple Macintosh versus the IBM PC and its clones. Macintosh publishing software and associated laser printers are strongly oriented to the PostScript file format, whereas IBM-family publishing software and laser printers are strongly oriented toward the Hewlett-Packard LaserJet Plus format. This situation is changing in the general direction of the more powerful PostScript format, which may become a universal standard for all types of desktop publishing hardware and software.

A clever and effective way to circumvent the output file format limitations of a given pageprinter is to provide printer emulation capability in the printer or in the personal computer, which means that the printer software contains code that allows more than one file format to be used. A HP LaserJet Plus printer can emulate a PostScript printer, and a PostScript printer can emulate an HP LaserJet Plus printer and any other dot matrix or letter-quality printer.

A page printed at a vertical and horizontal resolution of 300 dpi requires a substantial amount of memory to store the entire page. A quick calculation demonstrates this point. For an 8-1/2" by 11" sheet of paper, the dot density is (300)**2 = 90000 dots per square inch, or a total of 8,415,000 dots for complete coverage of the page. Each dot requires a single bit to turn it either black or white. Therefore, 8,415,000 bits, or 1.052 megabytes of memory are required. A byte (equals 8 bits) is the basic unit of memory. Somewhere, either in the personal computer or in the printer, this amount of memory must be available, or else the determination of the bit pattern to be printed must be computed in real time as the page is printed.

Portrait mode means that an 8-1/2" x 11" sheet of paper is printed normally, with the 8-1/2" edges horizontal. Landscape mode means that the paper is printed with the 11" edges horizontal. Portrait mode is used for manuscripts; landscape mode is used for tables, overhead transparencies and slides.

Scanners and Optical Character Readers

A scanner is any electronic hardware device that permits material in printed form, e.g., books, tables, typed manuscripts, printed advertisements, photographs, graphs, drawings, and labels, to be used in digital electronic format without having to be reprinted, redrawn, rephotographed, or retyped. Within the general category of scanners are three different types of hardware devices: (1) optical character readers (OCRs), (2) graphics scanners, and (3) facsimile (FAX) transmission machines. An optical character reader scans written text (alphanumeric characters) and converts the text into ASCII, EBCDIC, or IBM DCA character format strings that can be processed by computer software such as word processors, spreadsheets, data bases, and electronic publishers. A facsimile device digitizes images, whether graphics or text, into a bit-mapped format suitable for electronic transmission and reception over telephone lines. A graphics scanner digitizes photographs, drawings, and graphics into bit- mapped formats that can be edited and manipulated with computer software such as paint programs, hypertext software, windows, and electronic publishers.

All types of scanners use a scanner engine, which operates upon the physical principle that areas on paper with different percentages of white and black reflect different percentages of applied light. The reflected light indicates that the area is either all black, all white, or something in between, a gray scale. To operate a scanner, the text or an image to be scanned is illuminated and the reflected light measured typically with an electronic chip called a charge-coupled device (CCD), which basically is a light-sensitive multi-bit memory device. Charge-coupled devices are also used in video cameras, electronic still cameras, and as electronic receivers for telescopes. Measures of the quality of a scanner include the number of gray shades possible; the resolution, in dots per inch

(DPI); and the speed of scanning. The higher the quality the scanner, the more computer memory required to store a scanned image. A full 8.5-inch by 11-inch page scanned at 300 dpi requires 1.05 megabytes of storage. The processing of such images requires both substantial processing speed and substantial random access memory (RAM).

An extremely important consideration is the input file format (input relative to the computer) that scanner and OCR employ for the storage of bit-mapped and character-oriented information. For bit-mapped images, the objective is to store data in formats that are compatible with popular paint software, for example, Halo DPE, PC Paint, and PC Paintbrush Plus (for IBM-family machines and clones).

Closing Remarks

In this brief article we have outlined the major software and hardware issues in selecting ETP software for your personal use. Future articles in this series will address nontechnical and institutional issues.

Please write and tell us your views and experiences. We welcome your input to this discussion.

Appendix. Fonts and Typefaces

A font is defined as one complete set of characters in the same typeface and size, including letters, punctuation, and symbols. Examples of fonts are 12-point Helvetica, 14-point Helvetica, 10-point Times Roman, and 12-point Times Italic. A typeface (family) is a set of characters that have a basic stylistic foundation based upon attributes such as character weight (thin, medium, or bold), character width (condensed or extended), style (roman, italic, or oblique), and the presence or absence of serifs (serif or sans serif). A serif is a termination to a letter stroke, typically a line that crosses the main stroke of the letter that aids the eye in recognizing the individual letter. The text of this article is printed in 10-point Times Roman.

Fonts (a) may be resident in the printer (e.g., Apple LaserWriter), (b) may exist in the software package (desktop publishing or word processing), or (c) may be installed using a third party software (e.g., Bitstream Fontware, GoScript). In case (c), a font is defined as a set of characters made for a specific model of printer sharing a typeface, a type size, and a common set of attributes. Examples of character sets are US ASCII (95 characters), HP Roman 8 (190 characters) and PostScript (206 characters). Examples of attributes are character weight, character width, roman, italic, and bold. Each font is made using an installation kit supplied by the software house and stored on your disk. The font is downloaded to the printer when the user invokes it in the ETP software. Most typefaces are proportional: the character widths vary from one character to another. Three common typefaces among these - Courier, Letter Gothic and Prestige - are monospace: the character widths are all the same. Such typefaces are widely used in typewriters and computer printout.

Typeface families, for purposes of convenience, can be grouped into the general categories of text, display, or decorative. Text typeface families are used for reading, in the body of books, articles, and magazines. Display typeface families are designed to attract the eye and are used for short passages of texts, for example, titles, headlines, and signs. Decorative type families should be used with discretion in special situations where a highly formal (or sometimes informal) style is desired, for example, in wedding announcements. The minimum number of different typefaces should be used to accomplish a given printing job. A mixture of an excessive number of different typefaces visually jars the eyes and makes the document unpleasant to read.

One specialized typeface family that is used in a certain size for the creation of technical manuscripts is the family of mathematical and science symbols known as the mathematical pi font. For example, the Apple LaserWriter's symbol font is a mathematical pi font. Another example of a pi font is a chemistry-symbol pi font (available from Allotype Typographics).

It is easy to confuse the term font with the term typeface. The original Apple LaserWriter's 13 resident fonts represent only three different typeface families--Helvetica, Times, and Courier--available in a cumulative total of 13 different sizes called fonts. When one multiplies the total number of different typefaces by the total number of different possible typeface sizes, a very

large number of fonts can be created. If a typeface family can be defined by an algorithm or a mathematical formula, as is the case with PostScript, then a computer can readily scale it to different fonts.

Glossary

Bit map A graphic image formed by a matrix of dots with a specific number of dots per inch. Also called raster.

Clipboard Temporary storage for text or graphics under Microsoft Windows and other similar programs.

dpi Dots per inch

Font A complete set of characters in the same typeface and size, including letters, punctuation marks, and symbols.

Font face Bold, italic, underline or shadow.

Font size 8, 10, 12, ... points.

Footer One or more lines of text which appear at the bottom of every page.

Formatter A program to generate a file of printer commands which takes care of margins, font selection, centering, indenting, page numbering, filling, justification, hyphenation and footnoting.

Header See also Running Head.

Icon A functional graphic representation of a tool, a file or a command which is displayed on a screen.

Kerning Adjustment of space between letters in order to create visual consistency among all letters.

Landscape printing Horizontal text across 11 inch width of an 8-1/2 by 11 inch page.

Leading The amount of vertical spacing, expressed in points, between the baselines of two lines of text.

Markup language A language which describes a document and its components (paragraphs, sections, fonts, tables, charts, graphs, citations).

Optical scanner A device for converting an optical image to a dot matrix representation. A typical optical scanner produces a 300 dpi image. Higher resolutions are required for photographic images.

Phototypesetting Producing a page image on photosensitive paper. Sometimes referred to as cold type in contrast to the older method of casting characters, lines or pages in lead, known as hot type.

Pica A unit of measure equal to 1/6 inch, or 12 points.

Point The smallest unit of measure in typographic measurement. There are 12 points in a pica, and 72 points in an inch.

Portrait printing The normal printing orientation for a page: Horizontal text across the 8-1/2 inch width of an 8-1/2 by 11 inch page.

PostScript A page description (input) language for high resolution printer and typesetters

Resolution The number of dots per inch (dpi) used to represent an alphanumeric character or a graphic image. Typesetters print 1,200 dpi or more. Laser printers typically print 300 dpi or more. Screen displays are usually 100 dpi or less.

Running head One or more lines of text that appear at the top of every page of a document.

Style One of the variations within one family of typeface, such as roman, bold, italic, outline and shadow.

Style sheet A collection of type specifications and format definitions that can be saved and used in many different documents. Style sheets may be stored in separate files from the document (e.g., Ventura) or attached to the document (as in Interleaf).

TEX A widely used formatter which does not normally support graphics.

Text wrap The ability to wrap text around graphic images on a page layout.

troff A popular Unix-based formatter

Typeface A family of type which has a common, unified underlying design. Best known examples are Times, Helvetica, Courier and Palatino. Typefaces are broadly grouped into two categories: serif and sans serif. Times is a serif typeface; Helvetica is a sans serif typeface.

Vertical justification The ability to adjust the spacing between lines of text in fine increments so as to make columns end at the same point on a page and have pages end at the same point across a layout

Wrap See text wrap

WYSIWYG Abbreviation for "what you see is what you get"

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This article was prepared using Lotus Manuscript and printed on an NEC *Silent*writer.

Just-In-Time Publishing

By Peter R. Rony, Virginia Tech

At the exhibit associated with the recent Toronto ASEE meeting, the McGraw-Hill booth proudly exhibited a textbook, "Creative Problem Solving: An Introductory Course for Engineering Students," by Edward Lumsdaine and Monika Lumsdaine, an example of McGraw-Hill's "College Custom Series."

In chemical engineering, the problem with custom publishing may be that, because of the total sizes of our undergraduate and graduate populations, an individual faculty member may not be able to make the case that a custom-published ChE text would sell the required 500 to 1000 copies. Nevertheless, this is a positive and important development for all educators, and McGraw-Hill can be complimented on its willingness as a major publisher to pursue Just-In-Time publishing. Collaborative efforts, for example, those sponsored by CACHE, may well succeed in identifying custom material that would be widely accepted and adopted by domestic and foreign ChE departments. Also, custom publishing may complement expanding capabilities in Electronic Technical Publishing (ETP), discussed elsewhere in this newsletter; an author may no longer need to be responsible for writing a complete text, but could combine original writing with the Catalog of Current Database Items. Finally, the use of electronic communications could facilitate, among chemical engineering departments, the communication of the existence of custom published texts. Major publishers should establish Internet userids to facilitate two-way communications with faculty.

For further details about this program, please contact

Margaret Hollander,
Custom Publishing Editor
College Division
McGraw-Hill Publishing Company
Princeton Road
Hightstown, NJ 08520 (609) 426-5854

or a publishing colleague who many of us know,

B. J. Clarke, Executive Editor for Engineering
College Division
McGraw-Hill, Inc.
1221 Avenue of the Americas
New York, NY 10020 (212) 512-2012

The following is a direct quote from the McGraw-Hill brochure.

On the McGraw-Hill Custom Publishing System

The textbook will never be the same! McGraw-Hill's new Custom Publishing System will revolutionize the textbook industry by taking advantage of the latest advances in technology to give professors what they want: The ability to customize educational material to meet the specific needs of their students. And, at the same time, keep texts current with the latest advances in their fields, eliminate obsolescence, out-of-stock situations, provide greater teaching flexibility, save students money and increase convenience.

What is the McGraw-Hill Custom Publishing System?

It is a computerized publishing system that allows professors to select educational and professional information they need for their classes from a large, current database. McGraw-Hill will then paginate the material, create a Table of Contents based on the teacher's chosen organization, and personalize the cover of the new book with the name of the professor, class and course number, department, school, and location. McGraw-Hill will then print, bind, and ship the customized book to the school bookstore within days after receiving the order.

What are The Advantages:

The Custom Publishing system greatly expands professors' options and flexibility. Professors can custom design student material to match the specific needs of an individual course and even have different supplements for different abilities, or distinguish between majors and non-majors taking the same class. Texts can incorporate syllabuses and previously unpublished professor material, chapters from different texts as they are included in the database, as well as journal articles that are included in the "Catalog of Current Database Items." They are easily updated and,

therefore, can reflect the latest advances in subject areas.

Students will only pay for the material their professor wants them to use and will have all the materials needed for a course in one convenient volume.

The McGraw-Hill Custom Publishing System is the first Just-In-Time publishing system in history that provides a cost-effective alternative to traditional publishing. It also means no out-of-stocks, no out-of-print books, and more efficient distribution. All this and the ability of McGraw-Hill to strictly maintain the integrity of the copyright laws is a true revolution in textbook publishing.

Availability?

May/June to meet the demand for Fall 1990 classes.

What is Available?

The Meigs and Meigs text makes a powerful statement with regard to the capability of the system. Teachers of accounting require access to large amounts of teaching material, supplements, and accounting information. McGraw-Hill is the first publisher to respond to these needs by making available more information than ever before, and in a cost-effective, easy-to- use manner: The McGraw-Hill Custom Publishing System.

What Else?

The text of Meigs and Meigs will be available to teachers if they feel there is a need for a customized desk copy. Also, articles from periodicals such as "The Journal of Accountancy," and "Business Week," and financial accounting data. In addition, professors will be able to add their own syllabus or other important course materials.

What Will It Cost For Students?

There is a potential for significant savings! The price to students will be less if the professor requires less material. The student will only pay for what is used and needed in the course. For example, supplements will be pro-rated by chapter. Articles will have a set price per article.

Complimentary Copy?

Yes, professors can order a sample copy based on their needs. In addition, McGraw-Hill will make available a sample customized supplement to facilitate evaluation. A complimentary copy, with its own Book Number, should be carefully put together, for it can serve as the basis for the department or class order and prevent the professor from having to proof another copy, and therefore, save time in order fulfillment.

How Can A Professor Order A Custom-Published Product?

By filling out the order form for the desired chapter supplements, or later, texts, based on a catalogue provided by the sales representative. This form is then submitted to the bookstore with the regular book requisition for the text.

How Long Will An Order Take To Fill?

McGraw-Hill is committed to shipping an order within days of receiving it.

How Is Each Product Billed And Shipped?

McGraw-Hill generates the billing from its Hightstown, New Jersey facility. The book is sent by truck or UPS from Harrisonburg, Virginia. Customer pickup is available, as are other options as specified by the bookstore.

Future?

The "Catalog of Current Database Items" will be updated frequently as we expand the database offerings. Updates and revisions to previous information; more journal articles and new important financial accounting data; research in progress and other scholarly works; new applications, cases, practice sets, and problem sets; and new texts are only some of the items planned.

How the System Works: Stage One

McGraw-Hill's revolutionary custom publishing system makes use of a large database created using PostScript, the industry-leading page description language, and following standard McGraw-Hill editorial practices. These PostScript files of supplement chapters, journal

articles and financial accounting data are loaded at McGraw-Hill into a database on a workstation. Professors select from a Catalog of Current Database Items the material they want for their particular class and arrange this material in the order in which it is taught. After the professor's customized book has been verified and approved, the selection is processed by the bookstore, which places an order to McGraw-Hill in the traditional manner. McGraw-Hill confirms the order, does a credit check and, finally, transmits the order to the production facilities managed by R. R. Donnelley. The workstation at the production facilities makes use of software developed for McGraw-Hill by Eastman Kodak to "build a book" based on material selected by the professor from the McGraw-Hill database. The new customized book is paginated, a table of contents is created based on the selected order, and a title page generated with class and professor information. The book is printed, bound and shipped directly to the bookstore; shipping information is confirmed to McGraw-Hill, who in turn sends an invoice to the bookstore.

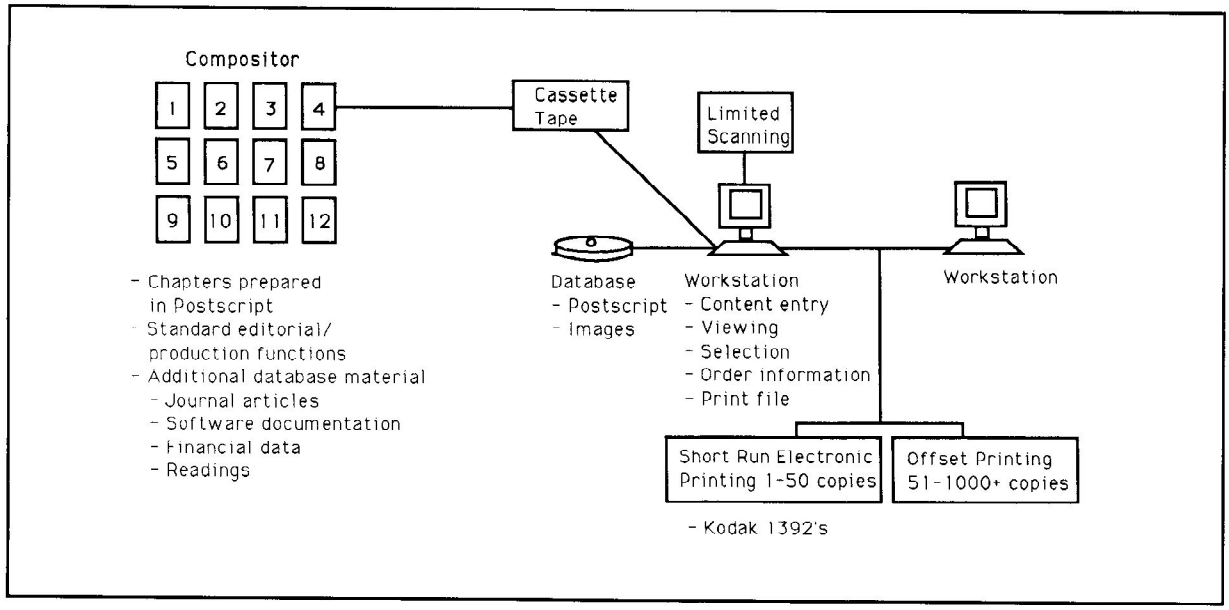
The Future: Stage Two

The future of the McGraw-Hill Custom Publishing System is just around the corner. As the illustrations below shows, plans are underway for the second and third stages. Part of the system will include the capability of a professor viewing the database on a computer workstation at the department office or at a local on-site publishing center. After viewing and approving selected contents from the database, the professor will have the opportunity to order this material in a customized book directly from a remote publishing center. The database will be stored in an optical storage device for easy and convenient delivery. The exciting possibilities of these capabilities are merely the next steps to the third stage of our plans.

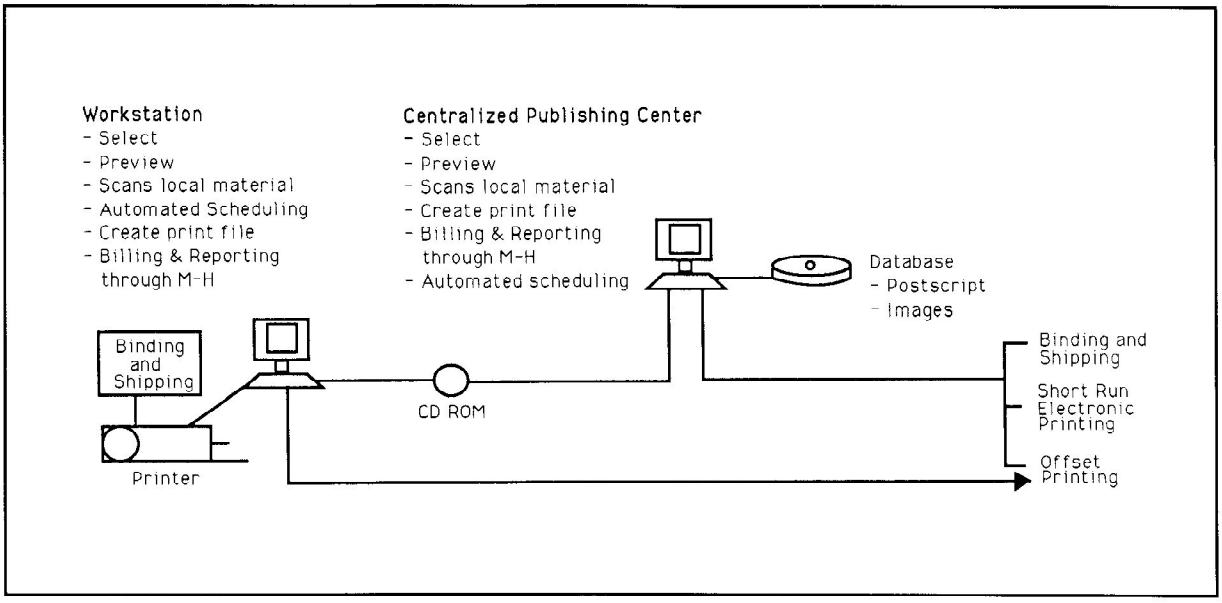
The Future: Stage Three

The third stage, but not the last, involves the creation of a distributed environment, where the database will be on-line, live to professors, students, and the local publishing centers. Professors and students will be able to interact dynamically with the material on the database, and professors will be able to order customized texts from McGraw-Hill or their local remote site for fast delivery of classroom material for use by their students. Ultimately, a total coordination of course material will be available for the classroom, the lab, and for home study.

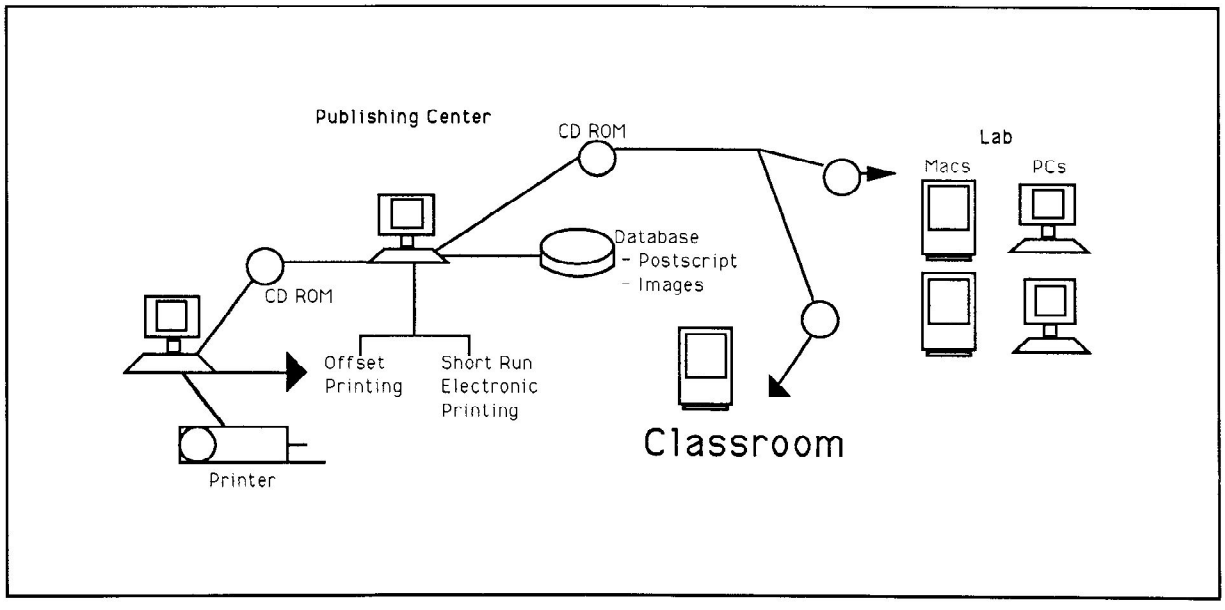
The printed book will never disappear, but will be greatly enhanced by the access to new, ever-changing information.



The Future: Stage One



The Future: Stage Two



The Future: Stage Three

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Chemical Process Engineering On Cray Research Supercomputers

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Supercomputers are transforming R&D activities in the chemical process industry (CPI). Companies in the pharmaceutical/biotechnology industry are using supercomputers to better focus and accelerate their R&D efforts in designing new drugs, vaccines, and herbicides. Large-scale molecular simulations of drug-enzyme complexes are used by researchers both to learn how a drug works on the molecular level, and to identify which of the many candidate compounds shows the most promise of being an effective drug. Further studies, requiring synthesis of the compound and experimental testing, can then be focused upon the most promising candidates.

The chemical and materials based industries are using supercomputers in a similar manner to obtain molecular based properties about their products and processes. Thermodynamic data, such as heats of formation and heat capacities, are being calculated on supercomputers, providing information which can often be too costly or time consuming to determine by experimental measurement. The molecular interactions involved in catalytic processes are being studied on supercomputers, yielding knowledge about chemical processes that are typically unobtainable by experimental means. Supercomputers are also being used to study the impact of chemical products on the environment, such as in the modeling of the global warming potential from chlorofluorocarbons. Polymer flows are being modeled using computational fluid dynamics methods to better understand and design injection molding processes.

More and more companies in the CPI are making the strategic decision to implement supercomputing as an integrated part of their R&D activities. Table 1 shows Cray Research's customers in the CPI, along with chemistry related research institutions. Cray Research also has nearly 30 customers in the petroleum industry, many of which are running chemistry and chemical engineering codes along with their traditional seismic and reservoir simulation applications. In addition, approximately 35 companies are using Cray Research systems for chemistry/chemical engineering at university and NSF-sponsored supercomputer centers.

During the second half of the 1980s, CPI application programs for supercomputers have improved substantially in functionality and performance. Industry standard codes in the areas of molecular dynamics, quantum mechanics, computational fluid dynamics, and structural analysis are available and optimized for supercomputer systems. The increase in the number of high- performance application codes has generated a growing interest in using supercomputer simulations for industrial research.

Surprisingly, until recently, there has been relatively little work done to develop or optimize application codes for large-scale chemical engineering design and optimization on supercomputers. However, initiatives at Cray Research, along with leading CPI companies, software vendors, and academic research groups, are signaling an end to this trend. We will discuss some of the chemical engineering design tools that are currently being tailored to run on Cray Research supercomputers and focus on the center of this application area, the process simulator.

Traditional sequential-modular simulators solve the material and energy balances of multi-component, multi-unit processes at steady state. The most widely used application codes in this area are PROCESS and PRO/II from Simulation Sciences and ASPEN PLUS from Aspen Technology. These modular codes are reliable and robust design tools with a long history of industry use and acceptance.

The CRAY version of PROCESS is currently running at about a dozen Cray Research customer sites. Version 4.0 is available from Simulation Sciences for running under both the COS and UNICOS operating systems. DuPont recently conducted an evaluation of PROCESS running on a VAX 8800 as compared to running on a single processor of their CRAY X-MP/28. In the October 1989 issue of Chemical Engineering Progress, Haley and Sarma reported that a single cpu CRAY X-MP increased performance on an average of 8 to 10 times over the VAX 8800. The

minimum ratio of CRAY to VAX performance was 1.9 and the maximum was 67.9. A cost analysis showed that the CRAY X-MP supercomputer was the more cost-effective solution. For DuPont users, the average cost per run on the CRAY X-MP computer is about half as much as on the VAX. It is important to point out here that many of the important PROCESS routines could have run significantly faster if they were optimized or redesigned for vector and multiple cpu operation. However, those involved in the project from DuPont, Cray Research, and Simulation Sciences chose not to pursue this since the follow-up to PROCESS, namely PRO/II, was due out in the near future.

PRO/II version 2.0.1 is already available for use on several personal computer platforms. In preparation for later CRAY releases, version 2.0.1 was ported to the CRAY X-MP and CRAY Y-MP running UNICOS. In June 1990, Cray Research obtained PRO/II 2.5.0 from Simulation Sciences. This is the pre-release of the official version 3.0.1, which will be released simultaneously for mainframe computers and CRAY supercomputers during the fall of this year. Cray Research plans to pursue a highly optimized version of the PRO/II simulator.

Cray Research has ported ASPEN PLUS 8.2-6 to the CRAY X-MP, CRAY Y-MP, and CRAY-2 supercomputers. The code is currently running at three Cray Research customer sites for four customers. The "official" ASPEN PLUS shell scripts are available on Cray Research UNICOS systems. These scripts are now in place for all variations of ASPEN PLUS runs (edit runs, user databanks, reusable load modules, etc.).

On the standard suite of 49 test problems from Aspen Technology, the unoptimized ASPEN PLUS 8.2-6 code was an average of 14 times faster on one processor of a CRAY Y-MP system than on a VAX 8530 mainframe. The speedups typically ranged between 12 and 17, but were as high as 25 and 32 for two of the test cases. It is important to note here that these 49 problems test various features of the ASPEN PLUS code and are not necessarily very computationally intensive.

Optimization work at Cray Research is well under way on the critical sections of ASPEN PLUS, which mainly include thermodynamic and equation solving routines. To date, over 20 routines have been optimized for vector operation. Six large ASPEN PLUS problems with VAX solution times ranging from 12 minutes to 4.5 hours have been obtained from Aspen Technology and a customer for use in Cray Research's optimization efforts. The speedup figures for the unoptimized and optimized CRAY Y-MP versions over the VAX 8530 version are given in Figure 1 for the six large flowsheeting problems.

Figure 2 demonstrates the impact of redesigning solution algorithms to fully exploit advanced computer architectures. Two large reactive distillation problems, RDIST1 and RDIST2, required about 90 minutes each to solve on the VAX 8530. A large portion of the total computation time was spent in the Harwell MA28 subroutine, which is a general sparse linear equation solver. This traditional solver was replaced with a new frontal solver. The motivation here is that the frontal routine exploits vector computer architectures by treating parts of the sparse matrix as full submatrices, thereby allowing arithmetic operations to be performed with full-matrix code (without indirect addressing). Using the frontal code, the total time required to solve these two problems in ASPEN PLUS was drastically reduced to only 1 minute for RDIST1 and 30 seconds for RDIST2. As a result, an engineer can now run this distillation model many times a day, instead of only once or twice. It should be noted that the frontal routine actually runs much slower on traditional sequential computers than MA28 because vector operations cannot be exploited.

A more detailed discussion on the use of the frontal code with ASPEN PLUS will be presented by S. E. Zitney at the AIChE 1990 Annual Meeting in Chicago. This paper will be part of the Symposium on Parallel Computing sponsored by Area 10C of the CAST Division.

Aspen Technology also produces Model Manager, a graphics front-end for the ASPEN PLUS program. With Model Manager, engineers can receive expert-system assistance to construct a rigorous flowsheet model. Later this year, a workstation version of Model Manager will be released. Similarly, Simulation Sciences plans to release an X-windows version of their PRO/II graphics package. This will enable the use of graphics workstations for the visualization of the flowsheet design process, coupled with the high-speed solution of the process simulation equations on a CRAY Y-MP. The result being a Network Supercomputing Environment which increases the abilities of chemical engineers to solve critical chemical process problems.

As noted above, chemical engineering computing is centered around the process simulator, but other related application areas include the simulation of physical systems (e.g., reaction kinetics modeling), linear programming (e.g., process scheduling), and dynamic simulation (e.g., startup and shutdown evaluation). Cray Research is also working to provide high-

performance solutions for these important design activities.

SIMUSOLV, from the Dow Chemical Company, is an integrated, multifunctional software package for developing and using

Table 1. Cray Research's Customers in the CPI

Installation	Customer	Machine
1986	Dupont	CRAY 1/A
	NCI	CRAY X-MP/28
1987	Scripps	CRAY X-MP/14se
	Dupont (upgrade)	CRAY X-MP/28
1988	Exxon R&E	CRAY X-MP/14se
1989	Monsanto	CRAY X-MP/116se
	Sumitomo	CRAY X-MP/116se
	Scripps (upgrade)	CRAY X-MP/116se
1990	Eli Lilly	CRAY-2S/2-128
	DuPont (upgrade)	CRAY Y-MP4/332

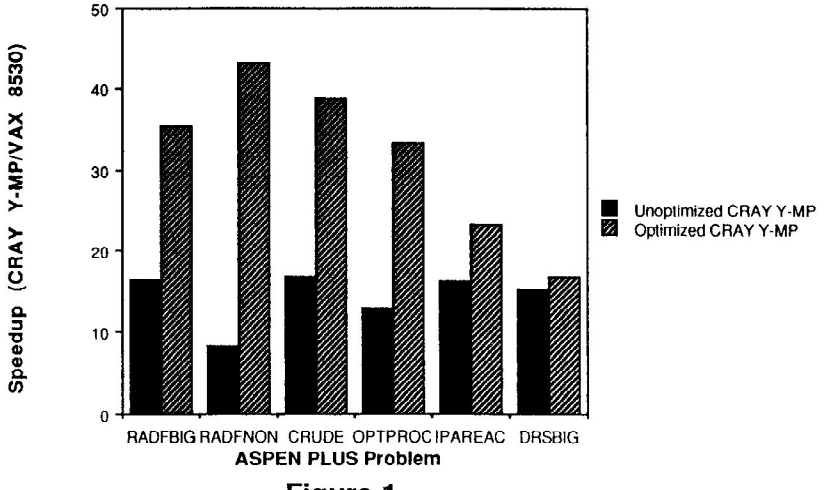


Figure 1

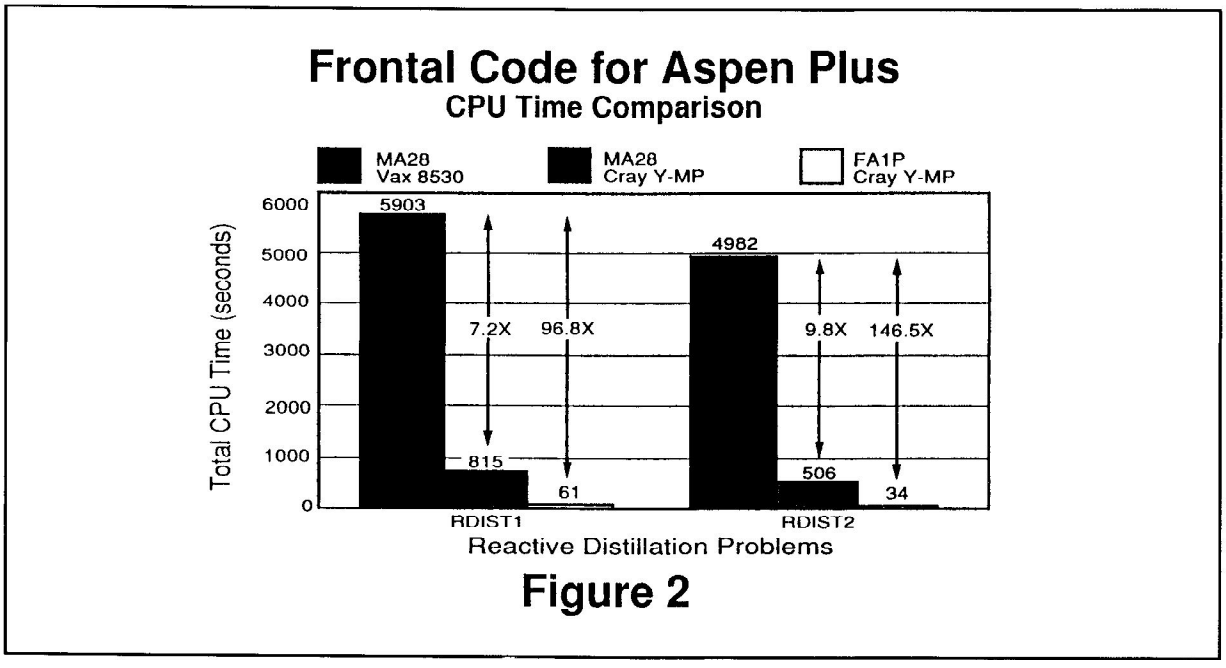


Figure 2

mathematical models of physical systems. This code can be used to model problems in such diverse fields as process engineering, toxicology, pharmacology, chemical kinetics, environmental sciences, and agriculture. In early 1990, Cray Research obtained the SIMUSOLV code for porting and has begun to optimize it for CRAY system architectures.

The General Algebraic Modeling System (GAMS) family of software is a complete system for modeling and solving optimization problems. A CRAY UNICOS version is supported and distributed by the GAMS Development Corporation. The system consists of: GAMS modeling language and execution system, and solvers for linear, nonlinear, mixed-integer, nonlinear-mixed-integer and nonlinear network mathematical programming problems. GAMS can be used in such CPI application areas as: process scheduling, retrofitting, batch processing, heat exchanger network synthesis and production, and distribution planning.

Cray Research is also investigating equation-based methods for solving chemical process simulation problems. The equation-based methods differ from traditional modular simulators in that they do not proceed sequentially from process unit to process unit in arriving at a final solution but instead treat the entire chemical process as one large equation set that is solved simultaneously. This approach allows for the efficient solution of problems involving dynamic batch and cyclic processing, startup and shutdown studies, control and operability studies, and operator training. Most importantly, the equation-based approach to process flowsheeting appears to be very amenable to the vector and parallel processing capabilities of Cray Research computer systems.

Many exciting challenges and opportunities for supercomputing simulations in large-scale chemical process synthesis/retrofitting, design/optimization, and operations/control exist. For example, there can be an enormous set of alternatives for the synthesis of a grassroots process design. The search space for a retrofit design can be even larger. But with the development of more powerful mathematical programming techniques, combined with increasing supercomputer power, it will become feasible to rigorously model, optimize, and automate the synthesis process. It is clear that there is profit to be gained by optimizing processes to run at some optimal point, but optimization is rarely performed on a whole process in the CPI. We expect that the ability to run large supercomputer simulations may bring process optimization, even optimization of entire plants having several different processes, into the arena of common industrial practice.

Connectivity between heterogeneous hardware is essential for developing an integrated process engineering environment. As network

supercomputing makes it possible, on-line use of supercomputer simulation models will help to ensure more efficient plant operation, both during normal operating conditions, and during changeovers and upsets. Cray Research will be continuing its efforts in meeting these challenges in order to bring these benefits to the CPI. In the near term, we foresee that the continued improvements in chemical engineering software for supercomputers will make process engineering on Cray Research systems a true partner to experimental efforts and pilot plant studies as the CPI strives to develop chemical processes that are more efficient, less costly to operate, and environmentally sound.

About the Cray Research Team...

We are always interested in hearing from others who are interested in supercomputing for chemical engineering. If you have any questions or comments, or would like further information on the work being done at Cray Research, please contact one of the authors.

Stephen E. Zitney joined the Industry, Science & Technology Department of Cray Research in June 1989 as a Senior Chemical Engineer. He earned his B.S.Ch.E. degree at Carnegie Mellon University and his M.S.Ch.E. and Ph.D. degrees from the University of Illinois at Urbana-Champaign. At Cray Research, he is involved in bringing the power of advanced architecture computing to the chemical process industry through the conversion, algorithmic analysis, optimization, and enhancement of large-scale, chemical engineering codes. His research interests include process synthesis, design, optimization, control, and scheduling. Phone: 612-683-3690, FAX: 612-683-3099, Email: sez@cray.com

Richard D. LaRoche recently joined Cray Research in May 1990 as a Senior Chemical Engineer with the Industry, Science, and Technology Department. He received a B.S. degree in Chemical Engineering from Montana State University and worked for two years with Dow Chemical before returning to graduate school. He earned his M.S. and Ph.D. degrees in Chemical Engineering from the University of Illinois at Urbana-Champaign. Dr. LaRoche joined the faculty at Penn State University in 1987 as an Assistant Professor of Chemical Engineering. He maintains affiliation with Penn State as an Adjunct Assistant Professor and continues to conduct supercomputing and parallel computing research for chemical process engineering applications at Cray Research. Phone: 612-683-3696, FAX: 612-683-3099, Email: laroche@cray.com

Robert A. Eades is the Manager of Chemistry Applications in the Industry, Science & Technology Department at Cray Research. Dr. Eades earned his Ph.D. in Physical Chemistry from the University of Minnesota at Minneapolis. He held positions at Argonne National Laboratory and Allied-Signal prior to his joining Cray Research in 1987. His interests and efforts at Cray Research are focused upon the development and application of computational methods to solve industrial based R&D problems in the fields of chemical engineering, chemistry, life sciences, and materials science. Phone: 612-683-3669, FAX: 612-683-3099, Email: eades@cray.com

About Chemical Process Flowsheeting on NSF Supercomputers...

ASPEN PLUS, PROCESS, and PRO/II can be made available for university instruction on CRAY systems at the NSF supercomputer centers at Illinois, Pittsburgh, and San Diego. In most cases, faculty can obtain instructional CRAY time by submitting a letter of request, instructor's curriculum vitae, course syllabus, and list of students. Students and faculty can access NSF supercomputers from their home campuses transparently through the use of the high-speed Internet networks such as NSFnet and associated regional computer networks. Each NSF supercomputer site can provide the necessary support and training to make your students' supercomputer use a rewarding educational experience.

Aspen Technology, Inc. and Simulation Sciences Inc. already provide their chemical process flowsheeting packages for university instructional use at a vastly reduced cost. These vendors can be contacted directly to obtain new or extend existing licenses to their software for use at NSF supercomputer centers. Listed below are the contacts to inquire about using ASPEN PLUS, PROCESS, or PRO/II on CRAY systems at the NSF supercomputer centers at Illinois, Pittsburgh, or San Diego.

To obtain further information about the Supercomputing Education Projects Program at the National Center for Supercomputing Applications (NCSA), contact: (on following page)

Dr. Nora H. Sabelli
Senior Research Scientist
National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
605 East Springfield Avenue
Champaign, IL 61820
Phone: (217) 244-0644
Internet: nsabelli@ncsa.uiuc.edu
BITNET: nsabelli@ncsagate

To obtain further information about coursework grants at the Pittsburgh Supercomputing Center (PSC), contact:

Wendy G. Janocha
Allocation Coordinator
Pittsburgh Supercomputing Center
4400 Fifth Avenue
Pittsburgh, PA 15213
Phone: (412) 268-5005
Internet: janocha@a.psc.edu
BITNET: janocha@cpwpsca

To obtain further information about allocations at the San Diego Supercomputer Center (SDSC), contact:

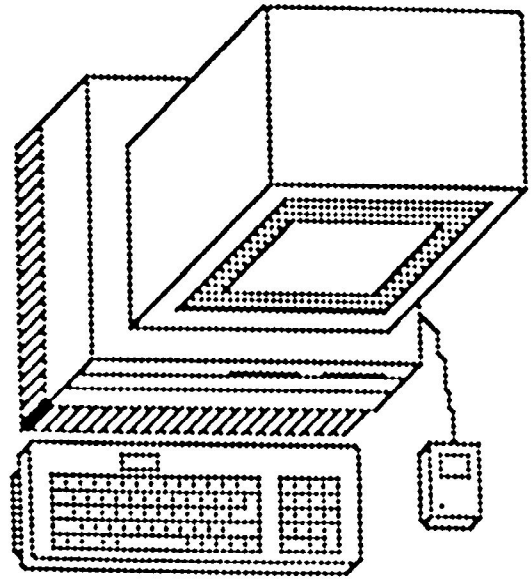
Rachel Chrisman
San Diego Supercomputer Center
P.O. Box 85608
San Diego, CA 92186-9784
Phone: (619) 534-5025
Internet: chrisman@sds.sdsc.edu
BITNET: chrisman@sdsc

For more information about the use of ASPEN PLUS at NSF supercomputer centers, contact:

Susan Palumbo
Aspen Technology, Inc.
251 Vassar Street
Cambridge, MA 02139
Phone: (617) 497-9010, FAX: (617) 497-7806

For more information about the use of PROCESS or PRO/II at NSF supercomputer centers, contact:

Linda L. Boyer
Simulation Sciences Inc.
1051 W. Bastanchury Road
Fullerton, CA 92633
Phone: (714) 879-9180
FAX: (714) 447-4107



Local Area Networking for Chemical Engineering Education

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Introduction

Chemical Engineering departments across the nation are in the process of expanding and updating instructional and research computing capabilities in response to the widespread changes brought about by new computer technologies. Networking has provided an efficient mechanism for the integration of new computational tools in both undergraduate and graduate curricula while exposing our students to the latest computer and networking technology in engineering research applications. Networking gives us the ability to provide easy access to a wide variety of computational tools that may reside on departmental and campus computers all the way up to systems at NSF supercomputer centers, other universities, and government laboratories. Even though we focus on networking issues as they pertain to research and instruction in chemical engineering academia, we believe our discussions will be of interest within the chemical process industrial community. No doubt the chemical industry is wrestling with many of the same concerns in creating an optimal working environment for the engineering professional.

In this work, we intend to provide an introduction to the power of networking for the chemical engineering student or professional. As we compiled information on networking technology, we reflected on how we obtained information in our quest to become familiar with networking issues. We realized that much of our learning process actually involved using the network as a resource for knowledge. This poses somewhat of a dilemma for the novice user since it seems that the most efficient way to learn about networking is to use networking. But how do you get started? It is our hope that this document will help the beginner gain access to networking techniques in a more efficient manner.

This paper can be divided into three major parts: network interconnectivity, local area network issues, and future networking opportunities. Our section on network interconnectivity gives the reader a bird's-eye view of how the Department of Chemical Engineering at Penn State University is linked to network resources at the campus, national, and international levels. The local area network section deals mostly with our experiences in setting up a local computing environment for instructional use. The wide area network section provides an overview of the worldwide Internet computer network and some of its applications. Finally, we summarize with some of our thoughts and speculations on where we see networking technology progressing as it applies to chemical engineering. We have included a network acronym section at the end of this paper to help the reader cope with the inescapable jargon.

Network Interconnectivity

Before getting into the specific aspects of our networking experiences, we want to provide an overview of the topology of network access for the Department of Chemical Engineering at Penn State. The Department of Chemical Engineering local area network (ChELAN) currently has 30 network nodes (listed below) interconnected on several segments of thinwire Ethernet coaxial cable. Ethernet networks support transmission rates up to 10 million bits per second (Mbps) on baseband coaxial cable. We are currently running network applications on the ChELAN which take advantage of both TCP/IP (Transmission Control Protocol/Internet Protocol) and DECnet network protocols. These communication protocols provide applications which allow data to be sent between machines in a reliable manner. Data sent from one network node to another are broken up into packets. The network protocols send and verify

receipt of data packets in addition to resequencing them if necessary.

Research Hosts

Machine	Ethernet Interface
1 IBM PS/2 Model 50	3Com 3C523
2 Apple Macintosh IIs	Kinetics EtherPort II
1 Digital VAXstation II	Digital DEQNA

Instructional Hosts

Machine	Ethernet Interface
8 AT&T PC 6300s	3Com 3C501
1 Apple Macintosh SE	Kinetics EtherPort SE
1 Digital VAXstation 3100 Model 40	Built-in Ethernet Interface
6 IBM PS/2 Model 30-286s	Digital DEPCA

Administrative/Faculty Hosts

Machine	Ethernet Interface
2 AT&T PC 6300s	3Com 3C503
1 DELL Turbo PC	Digital DEPCA
7 DELL System 200	Digital DEPCA

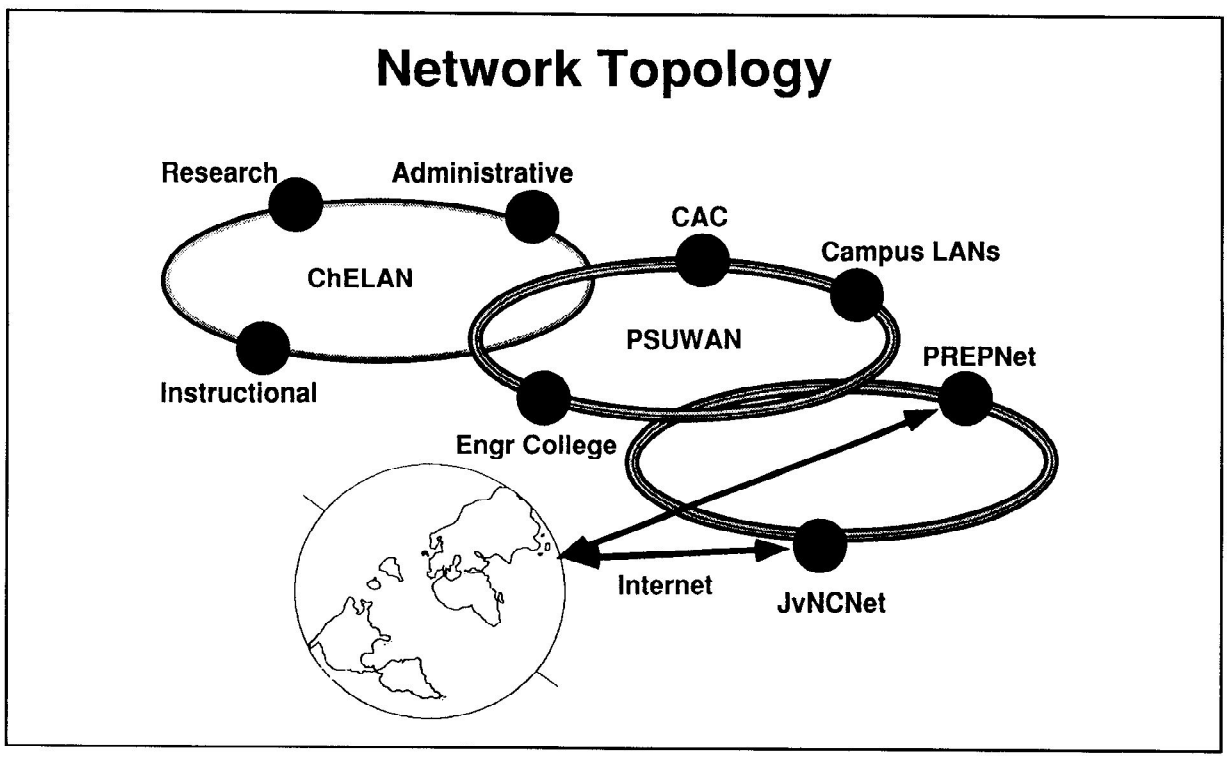

Figure 1

Figure 1 provides a conceptual view of how the ChELAN interconnects with other campus and national networks. The ChELAN is connected to a gateway computer which links the Ethernet-based local area network to the Penn State University wide area network (PSUWAN)[1,2]. The PSUWAN is a large-scale fiber-optic network which connects major buildings on the University Park Campus. The PSUWAN is based on the ProNET network protocol which supports transmission rates of 10 Mbps and 80 Mbps. The gateway computer has the responsibility of translating between the campus-wide ProNET and the local-area DECnet or TCP/IP protocols. The gateway computer provides routing service by checking for all ChELAN packets that are marked for network destinations outside the ChELAN. In addition, the gateway computer grabs ProNET packets on the PSUWAN that are earmarked for ChELAN network nodes.

The PSUWAN has connections to two larger scale TCP/IP-based networks, the Pennsylvania Research & Education Partnership Network (PREPNet) and the John von Neumann Center Network (JvNCNet). PREPNet is a high-speed network connecting a number of colleges, universities, and businesses within the Commonwealth of Pennsylvania. PREPNet is linked to the to the National Science Foundation Network (NSFNet) at the Pittsburgh Supercomputing Center (PSC). JvNCNet is another regional high-speed network which connects the members of the Consortium for Supercomputing, a group of universities in the Northeast associated with John von Neumann Center for Supercomputing (JvNC). JvNCNet still remains a funded computer network even though the NSF support for the JvNC supercomputer site at Princeton, New Jersey ends in 1990. JvNCNet links to NSFNet at Princeton. JvNCNet, PREPNet, and NSFNet use T1 transmission lines which are rated at 1.544 Mbps.

NSFNet spans the continental United States with major nodes at the National Center for Atmospheric Research (NCAR) and the NSF supercomputer sites at Princeton, Cornell, Pittsburgh, Illinois, and San Diego. Many regional networks connect into NSFNet at these major nodes. The entire national network of these regional networks coupled with the Defense Advanced Research Project Agency (DARPA) ARPANET is known as the **DARPA Internet** or simply **Internet.** Internet is the large collection of networks ranging from the smallest local area networks to the largest wide area networks which allows researchers to share information with colleagues across the country as easily as if they were in the adjacent rooms. Internet is designed to provide national networking capabilities for the scientific research communities with support from NSF, DARPA, Department of Energy (DOE), National Aeronautics and Space Administration (NASA), and other government agencies.

Internet connects over 30,000 computers at educational/research institutions, government organizations, and commercial organizations. Internet also includes several transoceanic and transcontinental satellite links. While Internet is largely based in the U.S., it has connections to other countries such as the United Kingdom, Finland, and Australia. We should expect that most major scientific and engineering research centers around the world will eventually be interconnected through Internet. Comer[3] provides an excellent overview and introduction to TCP/IP networks and Internet. Quarterman[4,5] gives extensive reviews of existing network and conferencing systems worldwide.

Benefits of Local Area Networking

The usefulness of a local area network revolves around the ability to share resources and data efficiently across a given workgroup. We wanted to promote the following major areas in the development of the Department of Chemical Engineering computer resources:

- File Transfer and Translation
- Software Accessibility
- Sharing of Limited Departmental Resources
- Security of Departmental Resources
- Consistent Graphical Interface

The ChELAN helped us to address these issues in our present needs while giving us the flexibility and structure to plan for increased future demands. The following discussion elaborates on how we employed the ChELAN toward these goals.

One of the obvious benefits of a local area network is the ability to transfer files between computers at relatively high speeds. Most often, we find that the rate-limiting step in network file transfers is the actual transfer of data to and from the computer's disk storage, not the Ethernet network. Network file transfers eliminate the need for the so-called sneakernet approach where the user runs down the hall with a floppy diskette of information. Network file transfer takes on broader applicability when coupled with file translation software. In this context, we are able to provide file sharing capability to users in a multi-vendor multi-media environment. Several products are currently available to translate files

between different applications running under different operating systems. Also, many vendors provide built-in translation capabilities in software packages which are supported on different computer platforms and operating systems. File translation coupled with high-speed file transfer breaks down barriers between a varied user community by providing ways for them to communicate more efficiently.

A local area network promotes software accessibility. It is possible to load software on a fileserver which can be accessed by many network users. This makes it easy to distribute public domain or site-licensed software. Software maintenance is an extremely time-consuming task when dealing with a large number of standalone computers such as in an instructional laboratory. Networking provides an efficient means to maintain and update software for a large group of users. We can link the local area network with other networks to actually receive updated software distributions electronically.

A local area network can be employed to share access to limited software resources. For instance, we would like to avoid buying a word processing package license for every computer in a student computer laboratory since we know that at any given time not all workstations will likely need to use the word processing program. To reduce costs while still remaining within the copyright restrictions, we could buy a smaller number of licenses, load the software on a network file server, and restrict the number of workstation connections to the software at the number of licenses owned. Therefore, the cost of providing software for students is greatly reduced. This arrangement allows access from a greater number of workstations as we maintain the terms of the license, namely using the software on one computer at a time per license.

Another benefit of the network is that it is possible to share limited output devices. It is no longer necessary to have a printer at each workstation. The workgroup has the flexibility to pool resources in order to reduce costs yet still maintain user access to a variety of output devices. This allows for greater diversification in the types of printers and other output units that can be made available to the network users.

We view the network as an important tool in maintaining proper security of Departmental resources. This security is provided by the ability to control write access to disks on a file server and make regular backups of software and data. Oftentimes, networks are viewed as leaving users susceptible to outside attacks from computer viruses and worms. Actually, when proper network security measures are employed, the risk of virus/worm attacks can be reduced. For example, ChELAN application software is protected on a network file server by allowing read-only or execute-only access by authorized users. The vulnerability to outside network attacks is usually curtailed by using the appropriate network and operating system security measures properly.

Finally, the local area network can provide a consistent interface for the user community. For instance, a friendly graphical interface (such as the X Windows System standard developed at Massachusetts Institute of Technology) can be used to allow the user to draw together diverse computing resources effortlessly from a single workstation. By using a standard graphical interface, we can make the network environment appear to be similar whether the user is using a MS-DOS microcomputer, an Apple Macintosh, or an engineering workstation running either VMS or *UNIX*.

Instructional Uses of the Chelan

The best way to look at the impact of networking on instructional computing in the Department of Chemical Engineering is first to discuss what was happening before the network was in place. Prior to network installation, we had several microcomputers available for instructional use. Attempts were made to maintain useful software on the standalone units. Software maintenance became an enormous undertaking. Software diskettes had to be produced and maintained for the machines without hard disk storage. Hard disk management was a never- ending chore for the rest of the machines. If left unmanaged, the hard disk machines would fill up with personal software and data which eventually made the instructional software difficult or impossible to use. Licensed software could not be protected from inadvertent or intentional erasures. These machines became software dumping grounds which severely impeded their instructional use in addition to providing a "breeding" area for computer viruses and worms.

This sort of situation resulted in much frustration for instructors, teaching assistants, and students. Instructors and teaching assistants had difficulty maintaining software for their courses. Students became frustrated with the inability to use the software they needed to complete class assignments. This environment was especially hostile to the novice computer user. Above all, novices need predictability and reliability from

the computers they use to develop computer skills. Novices couldn't help but feel completely lost and intimidated with our instructional computing situation. We concluded that an enormous software maintenance effort would have to be undertaken if our laboratory of standalone microcomputers were to be useful in Departmental instruction. It was clear that we either had to hire additional personnel to take care of these tasks or else find another avenue. We looked toward local area networking to provide us with a time-saving and cost-effective alternative.

As soon as our MS-DOS machines were networked, we were able to consolidate all instructional software on the Digital VAXstation fileservers. We made use of Digital's networking software with an X Window System interface to make it easy for the students to access course software. Figure 2 shows the graphical interface our students see when they turn on one of the laboratory MS-DOS microcomputers. All instructional software is immediately available to the student by pointing the arrow to the G: virtual drive icon and clicking the mouse. Each microcomputer station has read-only or execute-only access since the software is physically store on the VAXstation file server and protected through VMS operating system and DECnet network security measures. The user simply points to the application (s)he wants to start and double- clicks the mouse.

This first step in local area networking represented an enormous leap in instructional accessibility and usefulness. Instructional software became accessible to all users while at the same time it was protected against inadvertent and intentional tampering. The use of fileservers for shared software also frees up local hard disk storage on the individual microcomputers for temporary storage. Our hard disk management scheme for the individual laboratory microcomputers is simply to inform the users that these hard disks will be completely reformatted at regular intervals. We only need to restore the necessary files to connect to the network and to run standalone MS-DOS in case of network problems.

The graphical interface promoted novice user interaction. It literally became possible to sense computer anxiety levels falling as students were able to learn new computing skills efficiently and enjoyably. We also believe there was a significant psychological effect in the transition from standalone units to a network laboratory. Not only did these microcomputers become more useful for local computing but they became part of a larger, integrated computing facility. Users benefitted from access to shared printers, plotters, and disk storage.

We currently support storage and maintenance of Departmental instructional software on the VAXstation file servers. Development time is necessary to convert some programs to run effectively in the network environment, but this time represents only a minor fraction of the time which would be necessary to maintain software on standalone units. We have dramatically increased our efficiency by providing superior service with far less time demands on instructors and teaching assistants.

Another one of our goals is to provide as much access to productivity software (word processing, graphics, computation, etc.) as we can afford within budget constraints. We are fortunate that the Center for Academic Computing (CAC) at Penn State University provides many general-purpose microcomputer laboratories which fill most of the students' needs in these areas. Our philosophy is to provide enhancements geared specifically toward the needs of the chemical engineering student.

The connection of many departmental local area networks across the University Park campus of Penn State University has produced several avenues for more software services at less cost. In most cases, we prefer to arrange site license agreements with software vendors to give us the most flexibility. For example, Penn State University (through CAC) entered into an agreement with Digital Equipment Corporation for a site licensing and computer software distribution program for all VAX systems in the University. These initiatives are known as the Campus Wide Site License Grant Program (CSLGP) and the Education Software Library (ESL). CSLGP is a software licensing agreement which provides over 200 software license program authorization keys (PAKs) to authorized members of the program. ESL is a software maintenance and distribution agreement which provides over 40 software layered products to authorized subscribers of the program. Distribution of PAKs and software is accomplished electronically through the PSUWAN. In addition, CAC provides an electronic mail distribution system for news and technical announcement for subscribers to the CSLGP and ESL programs.

Many instructional programs fall into the site-license, shareware, or public domain categories where we are allowed to provide as many software copies as we deem necessary as long as the software is used for educational purposes. Such software can be loaded on the servers to allow access from any of the microcomputers on the network. If the licensing agreement permits, we can allow users to

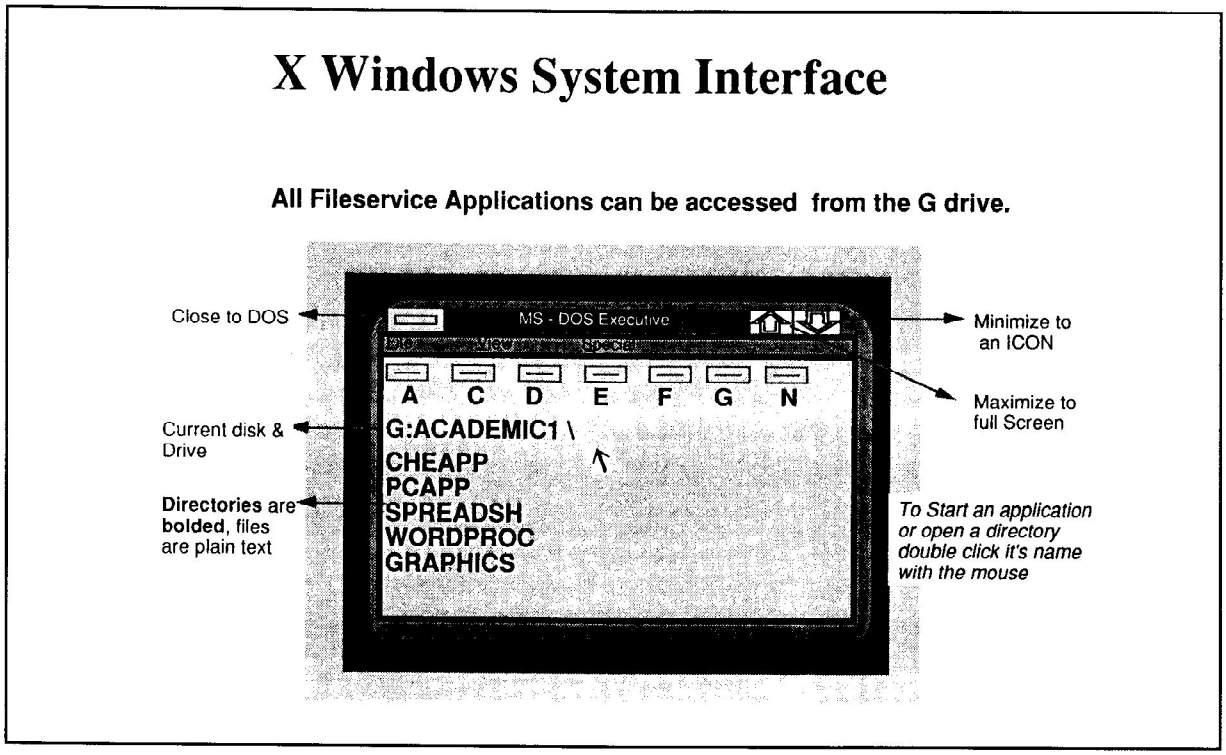

Figure 2

copy the software onto diskettes from the network so they can install the site-licensed software on their own personal computers. Our installation of the MicroMENTOR computer assisted software package from the University of Michigan is an example of site-licensed instruction software which is installed on the ChELAN. The MicroMENTOR System is explained in more detail in the courseware summaries later in this section.

In absence of a comprehensive site license agreement, software vendors usually license their software to be run on a single machine at one time per individual license. In many cases, it may be within copyright restrictions to put a software package on a network file server and limit network access. We may only need to buy enough licenses to cover the number of users which would need access at one time. We use the network to limit the number of simultaneous accesses to the number of licenses we have purchased. The network becomes a powerful tool to provide software access across a large workgroup while providing significant savings. In essence, we can take advantage of the fact that certain software packages may see only occasional use by a large number of potential users. The College of Engineering agreement with WordPerfect Corporation provides an example of software which we are allowed to add network accesses at a significant price reduction from standalone licenses.

In the next few sections, we briefly describe the instructional software packages which were used during the inaugural semester (Fall 1989) of ChELAN instructional operation. We discuss how local area networking enabled us to make an immediate effect in the quality of instruction for core courses in process design, mass transfer, process control, and thermodynamics.

ChE 401 - Chemical Process Engineering (required senior undergraduate course)

ChE 464 - Design of Chemical Plants (required senior undergraduate course)

Instructional use of the LOTUS 1-2-3 spreadsheet program is yet another example of how we use the ChELAN to provide services at a reduced cost. LOTUS 1-2-3 is used extensively by students in ChE 401 and ChE 464 for spreadsheet calculations involved in economic evaluation of chemical processes. It turns out that the most

efficient way to get the software in the hands of the students is for them to buy a special student edition of LOTUS 1- 2-3[6] at a vastly reduced price. The student edition comes complete with software and a manual for less cost than a typical textbook. Students often reported difficulties in setting up the software to obtain graphics output from spreadsheet calculations, however. We were able to use the ChELAN to assist the students in producing output by loading the appropriate LOTUS 1-2-3 device drivers for the instructional laboratory printers and plotters on the network fileservers. Students were relieved of the chore of setting up their printing environment. The user simply inserts the key diskette into a laboratory computer and double-clicks the 123.COM file on the graphical interface. In this fashion, we were able to provide students with network access to laboratory output devices for spreadsheet calculations while avoiding more expensive licensing arrangements.

ChE 413 - Mass Transfer Operations (required junior undergraduate course)

Our objective with this quality improvement project was to use local area networking as a tool to enhance the use of education software in the undergraduate curriculum. We sought to develop a straightforward methodology for efficient implementation of microcomputer courseware for use with chemical engineering undergraduate instruction. The MicroMENTOR software system was the first educational package installed on the ChELAN and was used extensively in ChE 413 during Fall 1989.

MicroMENTOR is computer-assisted-instruction software[7] developed in the Chemical Engineering Department at The University of Michigan for authoring and presenting mini-lessons called MicroMENTOR modules. MicroMENTOR is developed and distributed with the aid of the CACHE Corporation. CACHE (Email contact: cache@utxvm.bitnet) 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. Individual MicroMENTOR modules consist primarily of displays of text and graphics, execution of programs, and examination administration. A site license for the MicroMENTOR system has been acquired through the use of Departmental instructional funds. Existing MicroMENTOR modules are listed below.

Module	Application
MCCABE	McCabe-Thiele distillation
PONCH	Ponchon-Savarit distillation
BATCH	Batch binary distillation
CLASS	Steady-state process simulator (material balances only)
MATBAL	Chlor-alkali plant material balances
ROMBERG	Romberg integration
NEWRAP	Newton-Raphson nonlinear equation solver
RKFOUR	Runge-Kutta ODE solver
LINPRO	Revised Simplex linear programming
UNLP1	Nonlinear programming (Davidon-Fletcher-Powell & Broyden methods)

We used the MCCABE and BATCH modules to enhance the instruction of distillation design fundamentals through the use of several homework assignments. Additional homework exercises were prepared by University Scholar students which made use of the MCCABE, BATCH, NEWRAP, and ROMBERG modules. Each module provides the student with the opportunity to explore more complex mass transfer problems with extreme efficiency. In addition to providing the numerical tools to analyze such problems, these modules have on-line tutorials to help the student review fundamentals that have been presented in classroom lectures.

The MicroMENTOR system was chosen because it offers modules that are of interest to not only ChE 413 but also as supplements to several other undergraduate courses in the undergraduate curriculum. With the MicroMENTOR package, it is also possible to obtain statistics regarding the student use during the semester. Through the use of the network, examinations can be taken by the students on the networked microcomputers and stored on the fileserver for grading by the instructor and/or teaching assistant. We used this feature to give distillation homework quizzes during the course of the semester.

ChE 450 - Process Dynamics (required senior undergraduate course)

ChE 450 students used the CONTROL software package[8] developed at Clemson University. CONTROL allows for the development of simple feedback loop models, open and closed loop simulation, and simulated real time graphics of dynamic responses. It has built-in tuning packages which allow the student to quickly and easily compare various controller types and tuning methods.

This software package has made it easier for the students to learn the major concepts of the course. They get interactive and simulated real time experience in feedback control systems. It is easy to see the difference between open and closed loop response and among different types of controllers of simple processes. A student can also see the effects of lags and dead times on dynamic response.

Before the network, control was stored on the hard disks of three microcomputers. An average class size is 50 students which made it very difficult for the students to get adequate time to perform their work on the software. It was also necessary for the instructor to constantly make sure that the software was loaded and functioning properly on each of the machines. Now that CONTROL is loaded on the network fileserver, the software is available on all of the departmental machines and is easy to maintain. The students found the network easy to use.

ChE 524 - Chemical Engineering Applications of Thermodynamics (graduate course)

ChE 524 students used the VLE Standard Data Base & Models software package[9] developed at Penn State University. VLE is an interactive, menu driven program used to perform various thermodynamic calculations. The program allows the user to access any of 104 systems in the data base or to interactively input vapor-liquid equilibrium data for a new system. The user can test the data for thermodynamic consistency, determine the two-suffix Margules constant which provides an estimate of the ideality of the system, or obtain regression parameters for a number of the activity coefficient models and equations of state with several mixing rules. The program can calculate errors in the bubble point temperature, bubble point pressure, K-values, and relative volatilities.

The use of the network made it much easier for the instructor of this course to distribute the software to the students. This software package permitted the students to use and compare many VLE models for many different types of systems with ease. The success at the graduate level will undoubtedly lead to introduction of this software application in the undergraduate thermodynamics courses.

Future Uses of Networking

At our current stage of network development, we have only really taken advantage of local area networking tools for instructional computing. The use of LAN technology has been a tremendous success in promoting computer integration in our curriculum. We look forward to integrating our research experiences with Internet into the undergraduate and graduate curricula. Many exciting possibilities exist when we look toward linking our ChELAN up with the world of Internet. The ChELAN provides a window to a world of computing resources. The first logical step involves enhanced integration of campus mainframes and microcomputer applications. These interactions include the ability to quickly and easily transfer data between ChELAN microcomputers and campus mainframes in order to produce reports, spreadsheets, and graphics efficiently.

But why stop at just the campus level? As part of Internet, our ChELAN gives us the capability of using computing resources that may not reside on campus. From any computer on the ChELAN, we can use Internet to access computers clear across the continent as if they were just across campus! With this network technology, it has become straightforward to have a class of students use supercomputers available at one of the NSF supercomputer sites from the same environment they are accustomed to using for their normal classwork. We plan to expand the use of the ChELAN to use the resources available on Internet for instructional computing. In this way, we can bring cutting-edge computational tools into the classroom while educating our students in the use of networking technology. Many of these engineering computational resources might be beyond the abilities of a department (or even a university) to afford, but are available on Internet.

Today's engineering students already are forced to integrate a variety of computational tools on many different systems. Often they are given assignments involving mainframe packages and programming while they must produce documents making use of microcomputers. Their experiences are strikingly similar to the computing world of today's engineering professionals. Networking gives them the platform in which to integrate these resources efficiently. At the same time, they learn valuable

lessons of how to draw varied resources together toward the completion of an engineering task.

We would like to underscore that the networking environment we have created in the Department of Chemical Engineering is a result of fairly modest expenditures, by necessity. Given enough money, we have no doubt that any engineering department could provide computing solutions which will optimize the educational and research experience. Most of us, however, are faced with the task of creating such an environment on severely limited budgets. Through the effective use of networking, we have been able to incorporate a variety of modest microcomputers into a single computing resource which is immensely more valuable than the sum of its individual parts.

A major benefit of this strategy is that we have a continuous upgrade path. By this we mean that we extend the useful life of older equipment while still continuing to add new technology computers at the high end. We end up with a network environment where all the equipment is integrated in order to be more useful and productive than if each component stood alone. This is a multi-vendor environment where we can make the most out of our old microcomputers based on the Intel 8086 or 8088 microprocessors at the same time that we add fast, multi-user engineering workstations. Through the use of standard graphical interfaces, such as the X Window System, we can make the user environment look and feel the same across all network computers. In this manner, we can encourage the student to create and explore possible solutions to engineering problems.

Through either network hardware or software solutions, we can provide many additional ways to access software written for a particular operating system. One good example is the enormous amount of instructional software which is written for the MS-DOS operating system. We would like to make this software available to any network computer whether it runs the MS-DOS operating system or not. One possibility is to allow users on terminals and non-MS-DOS computers (such as Apple Macintoshes) to access a multi-user engineering workstation which supports a MS-DOS emulator. Another solution would be to attach a hardware device which supports several MS-DOS sessions via network terminal access. With either of these solutions, we can provide MS-DOS software access to a variety of terminals and computers on the network. A multi-vendor environment is encouraged while avoiding expensive individual machine solutions (such as co-processor boards in every Apple Macintosh).

Penn State University is implementing a network plan to accommodate future heterogeneous computing environments. For example, the College of Engineering is currently undertaking a major capital project which will give network access to every classroom, laboratory, and office within the College. All major trunk lines between and within buildings will be fiber optic cable to provide for future transmission rates of 100 Mbps using the proposed Fiber Distributed Data Interface (FDDI) standard[10]. With higher transmission rates, we can truly begin to use different network computers in a highly integrated fashion. Supercomputers can be employed on a numerical intensive application in conjunction with a specialized 3D graphics workstation for real-time visualization of physical phenomena.

As we look to the future of computing in engineering and science, it has become evident that workstations and networking will be central issues. We are quickly moving out of the age of the central mainframe computer as the sole basis of computational research and engineering. Rather, we will see scientists and engineers using many varied computation resources (supercomputers, engineering workstations, parallel computers, and microcomputers) all integrated through the effective use of networking technology. It will be this arena of distributed computing which will be the key toward true computer-integrated manufacturing and design of chemical systems.

Acknowledgments

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Network Acronyms

ACRF	Advanced Computing Research Facility located at Argonne National Laboratory

ARPANET	Advanced Research Project Agency Network
bps	bits per second
CAC	Penn State University Center for Academic Computing
ChELAN	Department of Chemical Engineering Local Area Network
CNSF	Cornell National Supercomputer Facility
CSLGP	Campus Wide Site License Grant Program for Digital VAX systems
DARPA	Defense Advanced Research Project Agency
DECnet	Digital Equipment Corporation proprietary network protocol
DOE	Department of Energy
ESL	Education Software Library for Digital VAX systems
FTP	File Transfer Protocol
JvNC	John von Neumann Center located at Princeton, New Jersey
JvNCNET	John von Neumann Center Network
Kbyte	one thousand bytes (eight bits per byte)
Mbps	million bits per second
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications located at the University of Illinois at Urbana-Champaign
NSF	National Science Foundation
NSFNet	National Science Foundation Network
PREPNet	Pennsylvania Research & Education Partnership Network
PAK	Program Authorization Key for Digital VAX system software
PSC	Pittsburgh Supercomputing Center
ProNET	Proteon, Inc. proprietary network protocol
PSUWAN	Penn State University Wide Area Network
TCP/IP	Transmission Control Protocol/Internet Protocol

Trademark Acknowledgments

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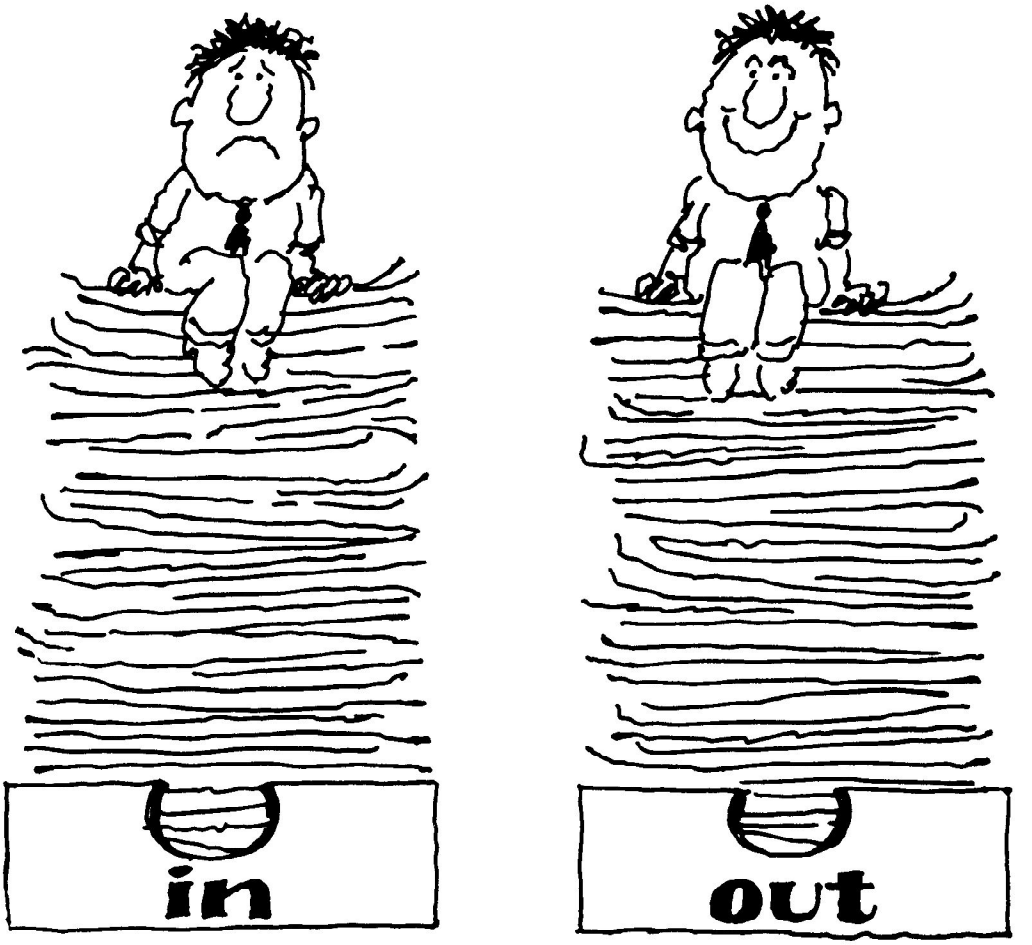

E-Mail Discussion Groups: A List Owner's Perspective

By Richard L. Zollars, Washington State University

E-mail discussion groups (mail lists) are nothing more than lists of names and e-mail addresses of individuals who have common interests in well defined topic areas maintained on a computer. The "list owner" is, in turn, the individual responsible for maintaining the list. There may be many reasons for establishing an e-mail discussion group but the most obvious is to provide a means of quick information transfer between a large number of individuals with similar interests. This information could be news of upcoming professional meetings, requests for papers, assistance on research problems or announcements of position vacancies. Anyone wishing to have such news distributed merely sends that item to the mail list and their message is copied and sent to all members. My initial goal in establishing the discussion group for interfacial phenomena (IFPHEN-L) was to make these services available to the members of area 1c of the AIChE.

Initiating a List

Actual implementation of the mail list was surprisingly easy. It started with what has been to date the most time consuming job: a mailing to all members of Area 1c in January, 1988 requesting e-mail addresses. After collecting the responses for five months I then contacted the computer center on campus to initiate the mail list. They put me in touch with the person whose responsibility was e-mail services. After some preliminary discussions I met with this individual for about two hours to discuss the operation of such a mail list, after which IFPHEN-L was born. At this point my only other responsibility as a list owner was to make sure that the expenses of operating the list were covered. These charges are minor and consist only of charges for the computer services used, such as disk storage of the list and the attendant records. Actual communication charges are free since this list is a part of BITNET.

Duties of the List Owner

After initialization, the responsibilities of the list owner vary depending upon how closely the owner wishes to monitor the list activity. As originally set-up, I elected to make access to IFPHEN-L as open as possible. Thus it was possible for anyone to subscribe, sign-off or send mail via the list without any action on my part. When operated in this fashion the list owner has essentially no day-to-day duties connected with the operation of the list. In addition, to attract new members a message was sent to various electronic bulletin boards announcing the formation of IFPHEN-L and inviting subscriptions. Unsolicited subscriptions via this route today account for approximately half of the current list membership (82 members total).

Operating in this fashion may relieve the list owner of many responsibilities but may result in other problems as evidenced both by my experience as a list owner and as a list member of other discussion groups. These problems can usually be traced to errors in the use of an electronic mailing list; the most common error being the different manner with which messages and administrative actions are handled. Most of the actions occurring within a list take place in the LISTSERV software resident on the machine that contains the mail list. The format of the command determines what actions LISTSERV takes with that command. Anything sent to a mail list is assumed to be a message which LISTSERV will copy and send to all members of the list. Administrative actions (subscriptions, sign-offs, requests for help or information, etc.) are distinguished from messages not only by the format used but also by the fact that they are sent directly to LISTSERV.

The problems that I have observed usually start when somebody mistakenly sends a message to the list. This message may be either an instruction which should have been sent to LISTSERV or a message intended for a single individual on the list. When received by the list, however, it is distributed to all members. This in turn elicits a response from someone on the list wondering why they received this message. Unfortunately, this response often goes back to the list, usually by using the "reply" option of e-

mail, so that all members of the list also receive this message. This is followed by other members responding in a similar fashion or members, annoyed at receiving these erroneous messages, trying to sign-off the list but mistakenly sending their requests to the list rather than LISTSERV, until the number of such "junk" responses becomes very large. (During a recent 24 hour period I received 33 such messages).

In all of the situations where I have seen this occur people began to sign-off the list because of the inconvenience of these periodic message floods. When this happened with IFPHEN-L, I felt that it was time to get more involved in the management of the list to prevent these problems. I again talked with the e-mail consultant at the computer center and rescinded many of the open aspects of the mail list. To other people communicating with the list, either to send messages or to subscribe, sign-off, etc, nothing has changed. Now, however, none of these actions occur unless I, as the list owner, approve thus allowing me to intercept erroneous messages prior to their distribution. I contact the senders of all messages that I feel were wrongly sent to the list to determine what their intent was. Since I have no desire to also serve as a censor for the mail list, all messages go to the list, regardless of their content, so long as distribution of the message is the intent of the sender.

By closing the open subscription option the number of messages that I receive as the list owner whenever the list is used was also reduced. When the first messages were sent over IFPHEN-L a large number of messages that I received as the list owner were notifications of incorrect addresses for list members. Although the command used by an individual to request subscription to the list remains the same, I now receive this message. To verify the address of potential subscribers to the list, I send a message back to the individual indicating receipt of their message. If within a 24 hour period I do not receive notification of a bad address I add the person to the list. Since implementing this change the number of incorrect address messages that I receive whenever the list is used has dropped to almost zero; the only exceptions are when an individual has moved but has not changed their e-mail address.

Time Requirements of a List Owner

While all of this sounds very time consuming it turns out not to be so. At the moment I receive approximately one to two requests per week for subscriptions and only about one message per month. Thus the time that I spend administering the mail list is less than an hour every month. I would prefer more business, especially in the form of more messages passing through the list. The volume of messages on this list does not appear to be atypical, however, as it is approximately the same on the other mail lists of which I am a member. The volume of messages does seem to have increased recently. These messages have to do with such topics as faculty openings, meeting and paper announcements and deadlines and requests for information on specific research problems. These were exactly the types of activities I had envisioned when the mail list was initiated and I am glad to see that it is being put to the use for which it was intended.

The Future

In the future, my hope is that the volume of messages will continue to increase. Membership on the list continues to grow from about 20 when the list was initialized a year and a half ago to 82 currently. Because of this increase in numbers I am also looking into additional services that might be made available through the list. The most obvious is a means of providing a bulletin board for storage of notices of future meetings and per deadlines.

While increased services and usage will also require more administrative time, I do not see these duties requiring unreasonable amounts of my time. By becoming moderately involved in the list administration I have reduced the overall time requirements by avoiding the need to deal with various emergency situations. This "preventive maintenance" type administration also helps prevent dissatisfaction by the list subscribers and insures the growth of the list. To others who are considering this type of activity my recommendation is to do it; knowing what I do now about list ownership I would do it again.

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!

THERMAL DESIGN OF SHELL AND TUBE HEAT EXCHANGERS

By Nurcan Bac and Ilker Ozal
Worcester Polytechnic

This program involves the thermal design of shell and tube heat exchangers conforming to TEMA specs. Propcty data bank and physical property estimation routines for 243 chemicals arc provided. Users have the ability to add or delete compounds. Physical properties of pure components, their mixtures and petroleum fractions are automatically generated.

Some of the methods used in property estimation are outlined below:

Property:	Method Used:
Vapor heat capacity	Empirical Constants Reid et al. (1977)
Liquid heat capacity	Bondi (1966)
Vapor viscosity	Stiel and Thodos (1962)
Liquid viscosity	van Velzen (1972)
Vapor thermal conductivity	Misic and Thodos (1961)
Liquid thermal conductivity	Reidel (1949)
Latent heat of vaporization	Pitzer (1955)
Saturated vapor pressure	Lee and Kessler (1975)
Surface tension	Brock and Bird (1955); Hakim (1971)

User friendly, menu driven software asks for the following inputs:

1. Project name and title.
2. Fluids involved, and their locations. Shell and tube side flowrates and pressures.
3. Shell and tube inlet temperatures, and outlet temperature of one stream, or heat duty, or temperature approach.
4. Allowable pressure drops, fouling factors, initial overall coefficient estimate, initial

geometry estimates (i.e. tube size, pitch, baffle spacing etc.) (Default values available).
5. Materials of construction.
6. Design pressures and TEMA class.
7. Chemical Engineering Plant Cost Index

The program performs Design or Rating tasks and optimizes the estimated fixed cost for the design case. The design mode also generates numerous alternatives with different geometry and cost. Summary screens indicate heat transfer and pressure drop details as well as cost estimates for plausible heat exchangers. Cost sorted lists and highly qualified specification sheets can be obtained for selected designs.

The program is developed during an M.S. thesis at METU Ankara, Turkey, and is useful in undergraduate heat transfer and design courses. The number of source lines are as follows : FORTRAN :4773, dBASE: 2853 , DOS (batch): 131 ; a total of 7757 . The program runs on PC XT/AT or compatibles and on 386 machines. MS-DOS 2.0 or higher and minimum 320 kB RAM is required. Display is either monochrome or color. The program comes in a 1.2 MB 5.25 in. disk , or two 360 kB disks with password protection, a user's guide, and a sample problem. A disk can be obtained for a donation of $ 22.00 by writing to:

Professor Nurcan Bac ,
Chemical Engineering Department
Worcester Polytechnic Institute,
Worcester, MA 01609.

OPTIMUM SERIES BIOREACTOR DESIGN

By Gordon Hill
University of Saskatchewan

This program computes the "best" possible design configuration for series bioreactors to achieve any desired substrate conversion. It is based on optimization theory and presently permits the user to choose one of four possible bio-growth models: i)substrate saturation (Monod), ii)substrate inhibition (Haldane), iii)product inhibition I (Aiba hyberbolic) or iv)product inhibition II (Ghose linear). The calculations are used in biochemical engineering courses and in process design projects which utilize continuous bioreactors.

The user of the program provides biokinetic and feed stream information in an input file. This includes the type of growth model, the maximum specific growth rate, yields, saturation constant, inhibition constant, feed concentration and final desired concentration. The program then evaluates the design strategy for a single CST bioreactor and the best design strategy for 2 series bioreactors. The user can then choose a final configuration (up to 10 series bioreactors). Typically, optimum designed bioreactors result in total processing volumes being decreased by factors ranging from 3 to 20 over a single CST bioreactor. In process design projects, this results in a significant drop in capital investment. Output is tabular in format and is sent to both the screen and to an output disk file.

The program is written in Turbo-Pascal and is provided in both source code and a math co-processor compiled version. A sample input data file and the corresponding best design strategy output file are also provided. A disk and descriptive information can be obtained for $12.00 (cheques payable to "University of Saskatchewan") by writing to: Professor Gordon Hill, Dept. of Chemical Engineering, University of Saskatchewan, SASKATOON, Sask. S7N 0W0, CANADA. Specify 3.5" or 5.25" & HD or MD.

EQUATIONS OF STATE

By Kenneth R. Jolls
Iowa State University

This program constructs three-dimensional views of thermodynamic PVT surfaces and process paths through interactive computer graphics. One first draws the PVT phase diagram for a pure fluid according to the ideal-gas, van der Waals, or Peng-Robinson equations. This produces a wireframe rendering of the surface by arbitrarily spaced lines of constant pressure, volume, and tem-perature.

Eight systems of units are available in the program as well as a variety of visual enhancements, including color and linestyle changes, two-dimensional end views, shaded borders, and pairs of diagrams drawn in overlay comparison.

With a PVT diagram in place, the user then adds one or more process paths from among the seven classical choices (constant P, V, T, S, U, H, or polytropic). Paths appear as curves on the 3-D surface connecting initial and final states. Property changes and heat and work amounts are given in the dialog output and are similarly available in several systems of units.

Data files for different fluids or for different treatments of the same fluid are prepared within the program and stored in the directory containing the program executable. A macro utility lets the user run (and prepare) pre-programmed command files that cause execution of various thermodynamic scenarios of interest. Several tutorial macros are supplied with the software. Equations of State is written in FORTRAN and is available for IBM-compatible micros having at least 640K RAM and EGA-level graphics. A math coprocessor is recommended.

Descriptive information may be gotten from:

Professor Kenneth R. Jolls
Department of Chemical Engineering
Iowa State University
Ames, Iowa 50011.

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, 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.

ANNOUNCEMENTS

New CACHE Design Case Studies

By Ignacio Grossmann, Carnegie Mellon and Manfred Morari, Caltech

The CACHE Design Case Studies Task force has published four different volumes over the last few years. The most recent case study, Volume 4, "Alternative Fermentation Processes for Ethanol Production" was developed by Professors Fournier and LeBlanc with their student Samer Naser at the University of Toledo in 1988. The interesting feature in this case study is that it involves the design of a flowsheet where different choices of fermentors have to be considered. Furthermore, this case study includes a floppy disk with input files for the simulator FLOWTRAN as well as a program written in BASIC to evaluate the performance of CSTR fermentors. This case study was developed as a response to the increasing need to expose students to non-conventional processes. An order for for this case study can be found in this newsletter.

In order to continue producing a greater variety of case studies, the task force is currently undertaking the development of three new cases studies that are described below.

Volume 5. "Retrofit of a Heat Exchanger Network and Design of a Multiproduct Batch Plant".

This case study, which has been developed by Richard Koehler and Brenda Raich at Carnegie Mellon under the supervision of Professor Ignacio Grossmann, should be available for distribution by January 1 (see order form in this newsletter). There will be sample copies of this case study at the CACHE Open House in the Chicago AIChE Meeting.

As opposed to the first four volumes, this volume contains two short case studies that can be developed by groups of 2-3 students in about two weeks. The first problem deals with the retrofit of a heat exchanger network consisting of 8 exchangers with 5 hot and 3 cold processing streams as well as steam and cooling water. The layout of the network and areas of the exchangers are also given. The objective is to determine a retrofit design that can reduce the energy consumption within specified limits for the capital investment and payout times. This involves analyzing different alternatives for energy recovery, matching of streams, addition of area, reassignment and/or removal of exchangers and piping. This problem can be used to illustrate concepts of heat integration, as well as the application of computer software such as Target II, THEN, MAGNETS and RESHEX.

The second design problem deals with the design of a batch processing plant that has to manufacture 4 different products, all of which require 5 similar processing steps (reaction, product recovery, purification, crystallization and centrifuge). An important aspect of this problem is that the production schedule and inventory must be anticipated at the design stage. Furthermore, this problem also requires analyzing alternatives for merging processing tasks into single units, and using parallel units with and without intermediate storage. The use of Gantt charts is emphasized to analyze different alternatives. The case study also includes two sets of homework problems that can be used to provide the basic background for the two problems.

"Chemical Engineering Optimization Models with GAMS".

This case study has been developed by Professors Larry Biegler (Carnegie Mellon), Chris Floudas (Princeton), Iftekhar Karimi (Northwestern) and Ignacio Grossmann (Carnegie Mellon) with their research students. This case study is currently under revision and should be available by the end of the year. Sample copies will also be available at the CACHE Open House in the Chicago AIChE Meeting.

This case study describes the formulation and solution of 21 chemical engineering optimization problems with the modeling system GAMS. While in the past optimization courses have been largely confined to small analytical problems, GAMS offers the possibility of solving a variety of meaningful optimization problems where the students can concentrate on problem formulation. GAMS consists of an an interface where optimization problems can be modelled in equation form. Indexed equations can be used to express models in compact form. Students need not be concerned with the details of interfacing optimization codes since this is performed automatically by GAMS. Also derivatives for nonlinear functions are generated automatically.

The case study includes the detailed description of problems in the areas of design, planning and scheduling of batch and continuous processes, chemical and phase equilibrium, design and synthesis of heat exchanger networks, distillation sequences and reaction paths, and optimization of dynamic models. Linear, nonlinear and mixed-integer optimization models are given at various levels of complexity; from textbook problems from Reklaitis et al. and Edgar and Himmelblau to recent research work in the area of process optimization. This case study should be useful for optimization courses at the undergraduate and at the graduate level. Special emphasis is placed on the formulation of models and excercises are given for each problem. The case study includes a special PC-version of GAMS, its user's manual and the input files to GAMS for the 21 problems. The GAMS software, which has been donated by GAMS Corporation to CACHE, includes the codes XA for LP and MILP, MINOS for NLP and DICOPT++ for MINLP. In addition, this case study includes supplementary material to show how GAMS can be used to implement solution algorithms for MINLP and optimization of differential/algebraic systems.

"Model Predictive Control with MATLAB".

This case study is being completed by Professors Yaman Arkun (Georgia Tech), Manfred Morari (Caltech) and Larry Ricker (Washington) with their research students. This case study should be available by January 1991.

Model Predictive Control (MPC) is a novel technique for feedback control which makes use of an explicit model of the process. It utilizes the model to predict the effect of manipulated variable moves and disturbances on the process output to be controlled. The manipulated variable is determined via on-line optimization such that the outputs behave in some desirable fashion. The major advantage of MPC is that interacting multivariable systems with time delay can be handled with ease and that constraints on inputs/outputs and associated variables are considered explicitly in the algorithm.

At present no tutorial introduction to MPC is suitable for its teaching at the undergraduate level. Work on a monograph in this area has been initiated by Carlos Garcia and David Prett at Shell and by Manfred Morari at Caltech. What makes the teaching of these techniques difficult is that they do not lend themselves to analytical study like classical control techniques, but that computer tools are required to communicate the main ideas to the students. In this case study an "MPC toolbox" has been developed around the commercial package MATLAB. MATLAB runs on most computer systems of relevance for education and is available at significant educational discount. The toolbox in this case study consists of a set of MATLAB macros that illustrate a variety of applications of MPC. A manual including several detailed case studies is being prepared to accompany the toolbox.

FEDIX: An On-Line Information Service for Universities and Other Research Organizations

By Peter R. Rony, Virginia Tech

At the session on "Computer Tools for Research Communications," Dr. A. Wohlpart, Vice President and Chairman of Oak Ridge Associated Universities gave a presentation entitled, "On-Line Databases for Federal Programs." In follow-up correspondence, he provided the Electronic Communications Task Force with a copy of DOE document DOE/ER-0423, "User's Guide to FEDIX" (Version 2.0, Release 1, October 1989). Given below are excerpts from this document.

1.0 FEDIX--General Information

FEDIX is a system of on-line databases providing information on Federal Government programs of interest to colleges and universities. The system currently contains information on the Department of Energy's energy-related equipment program, DOE research and development programs, faculty/student education programs, and DOE's minority assistance programs.

Databases containing information on Office of Naval Research and National Aeronautics and Space Administration programs will be developed in the fall of 1989 and will be available on-line in FY 1990. It is anticipated that other government agencies will soon be providing information on their programs.

1.1 Required Hardware

The system is not hardware dependent. The required modem setup is one stop bit, eight total bits, and parity check set to N for no parity.

1.2 Hours of Operation

The system is available 24 hours a day, 7 days a week.

1.3 Telephone Numbers

The two telephone numbers assigned to the system are,

- Computer (data) number:
  (301) 353-9520
- "HELPLINE" (technical assistance)
  number: (301) 353-9542

The HELPLINE (for problems or comments is manned Monday through Friday between 8:30 AM and 4:30 PM Eastern Daylight time, with the exception of federal holidays.

1.4 Accessing the System

1.4.1 Establishing a Connection

To establish a connection:

A. Configure your system according to the specifications indicated in section 1.1.

B. Dial the data line number via your modem or communications software. Your communications software displays the appropriate prompt when a successful data connection is made.

C. After a few seconds, the FEDIX "welcome screen" should appear on your terminal and you should be able to proceed with your session. If you encounter any problems, check your communication parameters with those specified in section 1.1 and retry the connection procedure from the beginning. PLEASE DO NOT HESITATE TO CONTACT US on the HELPLINE number if you require assistance with this procedure.

D. After the "welcome screen" appears, you will be prompted to enter your USER ID or to type the word "new" if you are a new caller.

1.4.2 First Time User

New callers must provide the following information to the system:

Enter your Name -- ex., Jon Doe: (32 characters maximum)
Enter up to a 6-character USER ID: (6 characters maximum)
Enter institution name: (32 characters maximum)
Enter your Department name: (32 characters maximum)
Enter street address: (32 characters maximum)
Enter city name: (16 characters maximum)
Enter state code: (2 characters maximum)
Enter zip code: (5 characters maximum)
Enter telephone number (999) 999-9999: (14 characters maximum)

Once the information is entered, the system re-displays the information you have provided and allows line editing. You may enter the line number of the information you want to edit, enter a '0' to re-enter all the information, or press <Enter> to accept all information and proceed. Your name and USER ID are required in order to register in the system. If you do not enter those fields, access to the system is not granted. Also, please remember your USER ID. It is required each time you access the system in the future.

The system then asks if you encountered any busy signals trying to access the system. You must enter an 'N' or 'Y' to proceed. If you entered a 'Y', the system prompts for a comment up to 20 characters describing the length of time or the number of times the system was busy (example, 4 times, 1 hour).

1.5 System Features

The FEDIX on-line system is designed to be very easy to use and provides a broad range of features for searching, scanning, and downloading. The easy-to-use menu-driven software will pose no problems for electronic information newcomers; experienced callers can use commands to bypass the menus.

The following special features will be useful in quickly and easily accessing databases.

1.5.1 Help

Help screens can be viewed from almost any menu in the system. To view a help screen related to a particular menu, just type "?" while at the prompt for that menu. The system searches the help database and, if a help screen is available, it is displayed on your terminal. If none is available, the system prompts for "HELP" to be entered to view an index of available help screens, press <Enter> to return. You may then request any of the available help screens to be displayed simply by entering the code for that help screen. This index of available help screens can be viewed from any menu simply by typing the word "HELP".

1.5.2 Menus

The system is organized by a comprehensive system of menus that reflect the organization structure of the information in the databases. It is a simple matter to go to any menu in the system by typing the two-character code associated with that menu and pressing <Enter>. A help screen is available that shows all menu codes.

1.5.3 Main Menu and Options

1.5.4 Capture

If you are using a microcomputer with communications software, it is likely your system is capable of capturing information as it comes across your screen. If you "turn capture on," you will be able to view information from the databases and store it in a file on your system, to be printed later. This may be desirable at times when downloading is not appropriate.

1.5.5 Command Language

A simple command language that can be used from any menu has been built into the system for experienced users. The commands take the place of going to a particular menu and selecting an option from that menu. For example, entering "LIST PROGRAMS" from the main menu is the same as going to menu [P] and selecting option 4, list programs. When any command is used, you always return to the menu where you entered the command.

For further details about FEDIX, including a copy of the User's guide, please contact:

Dr. A. Wohlpart, Vice President and Chairman
Oak Ridge Associated Universities
P. O. Box 117
Oak Ridge, TN 37831-0117
(615) 576-3255
FAX: (615) 576-0202

When asked about the use of BITNET to access FEDIX, Dr. Wohlpart responded as follows in July 1990: "I discussed with DOE the option of accessing FEDIX through BITNET. Cost to DOE is the main reason for not doing this. However, because there have been consistent requests along these lines, the issue is under consideration. One option being looked at is NSFNET."

1990-91 Electronic Database Files of Bitnet/Internet Nicknames

By Peter R. Rony, CACHE Electronic Communications Task Force
RONY at VTVM1
FAX: (703) 231-7826

The 1990-91 Chemical Engineering Faculties Directory will not include electronic mail userids. As Jim Rawlings (University of Texas, Austin) stated, "We decided to remove the email listings from the 90-91 directory to improve the directory's readability. We also felt that too many of the email addresses were incorrect and/or incomplete." As a consequence of this decision, the responsibility for creating and maintaining an electronic file of userids passed to the Electronic Communications Task Force of CACHE.

On August 11, 1990, a request was mailed to 157 domestic chemical engineering departments to supply the Task Force with (1) a single userid where broadcast electronic mail messages could be sent, and (2) individual faculty userids, specially those for faculty who actively used electronic mail. Each faculty userid was tested before inclusion in the nicknames file.

Each departmental and faculty userid was entered into a DBASE IV (version 1.1) file, FACULTY.DBF, which was then used to generate the variety of electronic and printed "reports" that chemical engineering faculty would use, for example, with IBM mainframes or VAX minicomputers.

For those departments that have access to the recently marketed DBASE IV (version 1.1), the parent FACULTY.DBF and related index and form files can be provided electronically. Note that DBASE IV runs on IBM PCs and clones.

Once created, the IBM nicknames file and the VAX alias file, based upon reports generated using DBASE IV, were sent to the University of Texas for inclusion in their CHELIB wide area network file server. Also sent was a complete listing of ChE departmental addresses (from the 1989-90 Directory), which is now available both as a DBASE IV file, DEPART02.DBF, and as an ASCII text file, DEPART02.TXT, that can be used with word processors such as Microsoft Word or WordPerfect. The 1990-91 Chemical Engineering Faculties Directory is currently in press; changes

to DEPART02.DBF and DEPART02.TXT will be made when the new Directory becomes available.

The next step in these efforts will be to add the Bitnet/Internet userids from international departments of chemical engineering. For further details about the University of Texas CHELIB file server, please refer to the "!NOTICE! Concerning Electronic Mail Addresses of Chemical Engineering Faculty" in this newsletter.

Status of Flowtran Load Modules for University Computers

By J. D. Seader, University of Utah

As part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to chemical engineering departments to install on their in-house computers. Thus departments would be able to run FLOWTRAN at no additional charge.

CACHE continues to supervise the preparation of FLOWTRAN load modules for some mainframe, supermini, and supermicro type digital computers and the distribution of the modules on magnetic tape to departments that order them. A new optimization feature is now included, and the instructional FLOWTRAN is in its third edition. Please see the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

Apollo workstations running AEGIS operating system (program on floppy disks).

CDC Cyber mainframe computers with the NOS operating system and a FORTRAN V compiler.

DEC VAX computers running with either the VMS or ULTRIX operating system.

IBM and IBM-plug compatible mainframe computers such as the 370, 30XX, and 43XX with the following operating system and FORTRAN compiler combinations:

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	OS/VS2 MVS	VS

Sun workstations running UNIX

Encore Multimax APC computer.

Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes, but not for consulting. A total of 176 FLOWTRAN tapes, cartridges, and floppy disks have already been distributed.

If you would like to obtain a FLOWTRAN tape for your computer and have not already contacted CACHE, complete and submit the FLOWTRAN TAPE form in the back of this issue of CACHE News. 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.

ADDENDUM

In "A User's Guide to Electronic Mail", an article in the last issue of CACHE News(Spring 1990), are listed the International DTE Communications Access Codes for 24 countries (Table 2, page 17). Yugoslavia did not appear in the list, so please note that Yugoslavia's DTE code is **2201** and Data Communication Network is **JUPAK**.

Foundations of Computer-Aided Process Design

Proceedings of the Third International Conference on Foundations of Computer-Aided Process Design
Snowmass Village, CO, USA, July 10-14, 1989.

edited by **J. J. Siirola**, *Eastman Kodak Co., Kingsport, TN, USA,* **I. E. Grossmann**, *Carnegie Mellon University, Pittsburgh, PA, USA, and* **G. Stephanopoulos** *Massachusetts Institute of Technology, Cambridge, MA, USA*
1990 vi + 568 pages, Price: US$ 195.00/Dfl. 395.00, ISBN 0-444-88233-2, Already published

Improved process engineering in general, and better process design specifically, hold the key to technology advancement in the chemical as well as biological, electronic, and other processing industries. This volume contains the proceedings of the Third International Conference on Foundations of Computer-Aided Process Design, which brought together engineers, scientists and graduate student researchers from a number of industrial, academic and government institutions throughout the world to assess and discuss the current status and future directions of computer aided process engineering.

The specific objectives of the conference were to provide a forum for an in-depth review of the current state-of-the-art in chemical process design as well as an introduction to process and product design in other disciplines, an evaluation of current and future needs in process design, a formulation of new research directions in computer-aided process design and an examination of educational needs in chemical engineering design. The nine sessions of the conference, presented here, focused on design theory and methodology, artificial intelligence applications in process engineering, chemical process synthesis, nonlinear systems analysis, batch and retrofit design, process engineering environments, chemical and nonchemical product design, recent process design research results and speculation on the future of process design.

It is hoped that the presentations, as reflected in these proceedings, will act as a bridge between established areas of design and design paradigms and new directions in design theory and methodology, and as a catalyst to foster an expanded scope of process design and its impact on product formulation, operations, quality, and economic robustness of manufacturing and processing systems.

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CACHE Process Design Case Study Vol. 4
Alternative Fermentation Processes for Ethanol Production

The objective of this case study is the preliminary technical and economic evaluation of a fermentation process for the production of ethanol from a molasses feedstock. The intent is to expose the student to some non-traditional chemical engineering processes and to the rapidly expanding field of biotechnology. Groups of 2-3 students should be able to complete the design in about 30 days. The major focus of this design study is the creation and rational development of a suitable process flowsheet, simulation of the flowsheet by a commercial process simulator (in this case FLOWTRAN), and economic evaluation and cost minimization of the final process.

The problem begins with the specification of the plant operating requirements. The type of fermentor to be used as well as plant operating conditions are left open. Suggested fermentors include batch, CSTR, CSTR with cell recycle as well as a novel extractive fermentor based on the use of hollow fiber membranes, the Hollow Fiber Extractive Fermentor (HFEF). The choice of fermentor will affect the nature of the flowsheet and lead to several design alternatives. Given the time constraints, the student will have to rationally screen these alternatives before arriving at a workable flowsheet ready for simulation. A kinetic expression describing the production of ethanol from glucose is provided as well as a 5 1/4" floppy disk (IBM format) with a BASIC program for evaluating the performance of the CSTR fermentors. Performance characteristics are also provided for the batch fermentor and the HFEF. Detailed explanations and graphics are included to explain the results and the FLOWTRAN program for the suggested design.

The problem statement was posed by Professors Steven E. LeBlanc and Ronald L. Fournier and prepared under their supervision, by Mr. Samer F. Naser, all of the University of Toledo.

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"Alternative Fermentation Processes for Ethanol Production"

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CACHE Process Design Case Study Vol. 5
Retrofit of a Heat Exchanger Network and Design of a Multiproduct Batch Plant

This volume contains two short design projects that can be developed by groups of 2-3 students in about two weeks. As opposed to the large projects that are commonly used in a design course, the objective of the case study is to expose students to a greater variety of problems and which are of current industrial significance.

The first problem deals with the retrofit of a heat exchanger network consisting of 8 exchangers with 5 hot and 3 cold processing streams as well as steam and cooling water. The layout of the network and areas of the exchangers are also given. The objective is to determine a retrofit design that can reduce the energy consumption within specified limits for the capital investment and payout times. This problem requires examination of alternatives for the level of energy recovery, matching of streams, addition of area, and removal or reassignment of existing exchangers and piping. This problem can be used to illustrate basic concepts of heat integration, as well as the application of computer software such as Target II, THEN, MAGNETS and RESHEX. The second design problem deals with the design of a batch processing plant that has to manufacture 4 different products, all of which require 5 similar processing steps (reaction, product recovery, purification, crystallization and centrifuge). An important aspect of this problem is that the production schedule and inventory must be anticipated at the design stage. Furthermore, this problem also requires analyzing alternatives for merging processing tasks into single units, and using parallel units with and without intermediate storage. The use of Gantt charts is emphasized to examine some of these alternatives. The case study also includes two sets of homework problems with solutions that can be used to provide the basic background for the two problems.

This case study has been prepared by the students Richard Koehler and Brenda Raich at Carnegie Mellon University under the supervision of Professor Grossmann who developed the problem statements and educational material.

CACHE PROCESS DESIGN CASE STUDY VOLUME 5
"Retrofit of a Heat Exchanger Network and Design of a Multiproduct Batch Plant"
(Available January 1, 1991)

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Salt Lake City, UT 84112
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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.

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: _____

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