CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 30

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

CACHE NEWS

No. 30	Spring	Spring 1990	

1 CACHE Curriculum Task Force

By Warren D. Seider University of Pennsylvania

9 A User's Guide to Electronic Mail, (Part 2)

By Peter R. Rony Virginia Tech

18 Partitioning of Pollutants in the Multimedia Environment: The SMCM Software

By Yoram Cohen, Wangteng Tsai and Steve Chetty University of California, Los Angeles

27 The Application Of Workstation Technology In Chemical Engineering

By Geoffrey Hulse The Ohio State University

32 CACHE Survey of PC-Based Flowsheet Software

By T. F. Edgar The University of Texas at Austin

35 Microcomputer Chemical Engineering Programs (developed by Professors)

Edited by Bruce A. Finlayson University of Washington

37 ANNOUNCEMENTS

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CACHE Curriculum Task Force

By Warren D. Seider, University of Pennsylvania

What is the role of computers in the chemical engineering curriculum? This, of course, has been a key question in chemical engineering education for the past three decades. In an attempt to respond when CACHE began in 1971, a Curriculum Task Force was formed, which set out to prepare computer problems and solutions (including FORTRAN programs) for the entire chemical engineering curriculum. Several additional task forces were organized, with more specific missions, including the Standards Task Force (to create standards for the FORTRAN programs being prepared by the Curriculum Task Force), the Large-scale Systems Task Force (to develop and distribute systems for the simulation of process flowsheets: e.g., FLOWTRAN), Thermophysical Properties Task Force (to develop and distribute programs for the estimation of thermophysical properties), and the Dynamic Systems Task Force (to develop and distribute programs for the dynamic simulation of process flowsheets and their control systems). In the ensuing years, many similar task forces were created to carry out specific projects (including the Real-time Systems Task Force, the Computer Graphics Task Force, and the Artificial Intelligence Task Force). The Process Engineering Task Force (which originated from the Large-scale Systems Task Force) has completed many projects and, like the Curriculum Task Force, has remained in existence since the inception of CACHE.

Throughout its 20 year life, the mission of the Curriculum Task Force has varied somewhat, but its perspective has remained broad. The Curriculum Task Force, together with the task forces it has spun off, has attempted to address the broader curriculum issues. Some have called for it to maintain a living position paper in which the

Task Force Members



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Stacy G. Bike is the Dow Corning Assistant Professor of Chemical Engineering at the University of Michigan. She joined Michigan in 1988 after receiving her B.S., M.S., and Ph.D. in Chemical Engineering from Carnegie Mellon University. Her research interests are in the area of colloid and interface science focusing on the role of colloidal forces in the processing and transport of colloidal systems. Two ongoing research projects are the development of a novel light-scattering technique to measure colloidal forces and the characterization of rheology-control agents. Together with Ignacio Grossmann of CMU, she coauthored a CACHE Process Design Case Study. She is also a co-principal investigator in the NSF/CACHE initiative "A Focus on Developing Innovative Engineers" and has supervised the development of a computer simulation for an introductory chemical engineering course.



Brice Carnahan is Professor of Chemical Engineering at the University of Michigan. His computing interests are oriented toward mathematical modeling, design of engineering and instructional software, and numerical methods (he is coauthor, with H. A. Luther and J. O. Wilkes of the Wiley text, Applied Numerical Methods). He served as Director, Vice-chairman, and Chairman of the CAST Division, and was recipient of the CAST "Computers in Chemical Engineering" Award in 1981. He developed the MicroCACHE CAI system (made available through CACHE in 1985), and has recently released the MicroMENTOR software (for IBM PC's and compatibles) for networked management and delivery of virtually any application program (including, for example, Unison modules); the package also includes authoring tools for creating instructional modules, and several chemical engineering and numerical methods modules prepared using the software. He has been awarded the ASEE 3M Lectureship for 1990.

role of the computer in all aspects of the curriculum is documented and upgraded regularly as computer hardware and software developments unfold at a rapid pace. However, as this article will reveal, the projects of the Curriculum Task Force have fallen short of achieving this objective for several good reasons.

Computer Problems for Seven Core Courses

In the first three years of CACHE, the Curriculum Task Force, under the direction of Prof. Ernest J. Henley (Houston), prepared seven volumes of computer problems for use in the core courses of the chemical engineering curriculum; material and energy balances, thermodynamics, transport processes, kinetics, stagewise processes, process design, and process control. These volumes, comprised of 125 computer problems, provided supplementary problems for use throughout the curriculum. They were widely distributed and moderately used, mostly in the design and control courses.

AIChEMI Modules

Upon completion of this project, the task force shifted to the preparation of single-concept modules for instruction in the core courses. Profs. Henley and David M. Himmelblau (Texas) coordinated the preparation of 250 AIChEMI modules which have been distributed by the AIChE for the past decade. An attempt was made to convert these modules into machine-readable form for distribution in a database for the PDP 11/23, but this effort was aborted for lack of financial support (after nearly 50 percent of the modules had been converted). Aside from this, it is noteworthy that the project involved no computation.

Task Force Reformulation and Accreditation Guidelines

In 1984, the Curriculum Task Force was reformulated with a mission not to define a model curriculum, primarily because "the manner in which the subject matter is distributed within a curriculum is highly dependent on the interests of the individual faculty and local constraints, as



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Morton M. Denn is Professor of Chemical Engineering at the University of California at Berkeley. He received his B.S. degree at Princeton University and his doctorate from the University of Minnesota. From 1977-1981, he was the Allan P. Colburn Professor at the University of Delaware before moving to Berkeley in 1981. Mort served as cochairman of the CACHE Curriculum Task Force from 1984-1985. He is currently the editor of the AlChE Journal. His research interests are in the area of polymeric materials.



Thomas F. Edgar is Professor and Chairman of Chemical Engineering at the University of Texas, Austin. He received his B.S.Ch.E. from the University of Kansas and the Ph.D. in Chemical Engineering at Princeton University. Dr. Edgar has been President of the CACHE Corporation, Chairman of the Computing and Systems Technology Division of AlChE, and President of the American Automatic Control Council. He has won the AlChE Colburn Award and the ASEE Westinghouse Award. He has served on the editorial boards for Chemical Engineering Reviews, Computers and Chemical Engineering, and the AlChE Journal. Dr. Edgar has published extensively in the fields of process control, optimization and mathematical modeling and is author of Coal Processing and Pollution Control, and coauthor of Optimization of Chemical Processes and Process Dynamics and Control.

well as the accreditation requirements." However, it was determined that CACHE should attempt to influence the content of the curriculum as well as to provide guidance to the AIChE and ABET with regard to the appropriate accreditation guidelines. To achieve this, a position paper was prepared and revised in response to the criticisms of the AIChE Education and Accreditation Committee. These guidelines, which were adopted by the E & A Committee as recommendations to the ChE Departments, are presented in Table 1.

IBM PC Compatible Lessons for Courses Other Than Design and Control

Also in 1984, because computing technology was being used principally in the design and control courses, few new initiatives were deemed necessary here, especially since the Process Engineering Task Force was involved in distributing steady-state and dynamic simulators for process flowsheets, programs for heat integration, and programs for process synthesis, among other software packages. Rather, the potential need for more effective usage of computing technology in the other core courses was recognized. This resulted in the first of two projects to prepare and distribute microcomputer lessons.

In the Fall, 1987, six lessons for the IBM PC (and compatible PCs) were distributed by CACHE. These lessons are listed in Table 2. They

were intended to provide supplementary exercises for the core courses, while providing students with opportunities to solve open-ended problems throughout the curriculum, and not just in the design courses. A booklet of diskettes was circulated to over 120 departments that support CACHE and to many others around the world.

All of the lessons were prepared to be compatible with the core chemical engineering courses: stoichiometry, transport processes, reaction engineering, thermodynamics, etc., and to be independent of the use of any particular textbook. The lessons utilized software provided on floppy disks and implemented on the IBM PC, for the most part, using the BASICA programming language with a color graphics monitor. No other restrictions were set, and consequently, several different formats evolved, some using extensive color graphics with animation to present new concepts, some presenting a derivation of the principal equations (with interspersed questions to be answered by the student), and most permitting parametric studies with graphical output.

These IBM PC lessons were developed, for the most part, on an experimental basis, often by student programmers, with little or no remuneration. Yet they presented examples of what could be accomplished with highly-interactive microcomputers, and provided the authors experience in the preparation of CAI software. (continued next page)



Bruce A. Finlayson is the Rehnberg Professor and Chairman of Chemical Engineering at the University of Washington. He received his undergraduate education at Rice University (1961) and his Ph.D. from the University of Minnesota (1965). He served in the Navy for two years and then began his teaching career at the University of Washington. He has been active in CACHE and CAST since 1981. He writes microcomputer programs for educational uses and edits the section of CACHE News for announcements of microcomputer programs written by professors.



H. Scott Fogler is the Vennema Professor and Chairman of the Chemical Engineering Department at The University of Michigan. His research interests are in flow and reaction in porous media, colloid stability, wastewater treatment, and dissolution kinetics in microelectronics fabrication. He is author of two books and over 100 research publications. His most recent book, The Elements of Chemical Reaction Engineering, was published by Prentice Hall in May of 1986 and has been adopted at over 100 universities. For the past 22 years, Scott has been a consultant for Chevron Oil Field Research Company. In 1980, he was a first recipient of the newly instituted award for Outstanding Research from the University of Michigan College of Engineering. In 1987, he received the University of Colorado Distinguished Alumnus Award, and in 1988, he was elected President of CACHE.



Ernest J. Henley is Professor of Chemical Engineering at the University of Houston. He received his B.S. degree from the University of Delaware and his M.S. and Dr. Eng. Sci. degree from Columbia University. Ernie was a trustee of CACHE from 1971-1981 and president of CACHE in 1974.

UNISON Authoring System

The limitations of the BASICA language and the lack of utility routines for creating the menus, text screens, graphical screens with animation, quizzes, etc., were well recognized by the end of the project. In one case, this resulted in 1200 hours having been expended to prepare interesting and challenging sequences which use color and animation, avoid repetition, give the students much control, etc.

In parallel, several authoring systems were being developed in which these and other utility routines were provided for the authors of CAI lessons. The task force evaluated several of the authoring systems and selected UNISON (a Courseware Applications, Inc. product) for its next set of PC lessons (to be discussed below) primarily because of its MacIntosh-like graphics capabilities. We were especially impressed by the ease with which annotated graphics displays could be created.

Factors Impeding Computation in the Transport, Thermodynamics and Reactor Courses

It is well recognized that computers are not used often in many of the core courses, especially in the fluid mechanics and thermodynamics courses. Computer programs have been slow to be developed and accepted as supplements for these courses, and the CACHE products in these areas

are not utilized often, including the recent IBM PC lessons. The underlying factors are probably closely related to the preference of the faculty to derive equations and illustrate the basic concepts at the chalk board, assigning homework problems involving models that are challenging to formulate, but with simple solutions (often analytical) that require little computation. Instructors in engineering science courses (often among the best in chemical engineering) seem satisfied that they can teach the concepts effectively without computation. They argue that the disadvantages, which often include the need to write programs, the rigidity of canned packages. the time extracted from crowded curricula, and the increased preparation time, outweigh the advantages. The new PC lessons suffer less from these disadvantages, but often these are rejected partially because they fail to utilize the ability of the computer to be highly interactive and present animated images that extend the ability of textbooks to describe the basic concepts.

All of the PC lessons enable the students to carry out parametric studies and display the results interactively, usually using graphics. Some are especially well-designed to permit open-ended problem solving, often with an economic objective function. Still, many faculty with an engineering science orientation do not welcome these supplementary materials as a vehicle for introducing design-oriented, open-ended problems in their courses. (continued next page)



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Deniz Karman is Professor and Chairman of Chemical Engineering at the University of New Brunswick. He received his B.Sc. degree from the Middle East Technical University and M.Sc. degree from Ege University, Turkey. He has been teaching at UNB for 12 years, after receiving his Ph.D. there. His interests in curriculum development have been in the integration of computer aided design packages throughout the curriculum, development of microcomputer based data collection and analysis applications in the undergraduate laboratorics, and developing computer aided instruction modules.

Page 4 Spring 1990

IBM PC and PS/2 Compatible Lessons in Fluid Mechanics

Despite these obstacles, the Curriculum Task Force is preparing five IBM PC and PS/2 lessons for the fluid mechanics course. These are listed in Table 3. When completed later this spring, they are expected to provide better teaching materials through the use of faster computers with more memory, higher-resolution displays, and the UNISON authoring system. Furthermore, all five lessons are devoted to the same course and, although they represent just a small sampling of the potential lessons in fluid mechanics, they provide a sufficiently large number to be considered seriously by instructors in fluid mechanics.

It is noteworthy that a similar concentration of 8 PC lessons for the chemical reaction engineering course have been well-received. These modules, used in conjunction with "Elements of Chemical Reaction Engineering" by H. Scott Fogler, have been purchased by 50 ChE departments.

PC Modules for the Development of Innovative Engineers

In a related project, with NSF support, the University of Michigan's chemical engineering department has undertaken to enhance innovation in its core chemical engineering courses through the development of open ended problems together with interactive computer modules and problemsolving heuristics. The open-ended problems are representative of those encountered in industry and

involve, for example, the use of lasers to melt and cut videotape, methods for crystallizing Si crystals and slicing Si wafers, the addition of vitamins to cereal, and the manufacture of optical fibers, among many others. Three to five interactive computer simulations are being prepared for each of five chemical engineering courses. By providing a large number of branch points, the students' decision making and divergent thinking skills are exercised. Each menu-driven simulation is being developed to review the fundamentals, provide a demonstration, followed by an interactive exercise that couples branching decisions with the problem solution and an evaluation of the students' performance.

This project has the potential to develop a host of computer modules on a much larger scale than has previously been attempted by the Curriculum Task Force. It should significantly add to the courseware to be distributed by CACHE.

Graphical Computer Aids for Chemical Engineering Education

For the past few years, the Curriculum Task Force has been attempting to initiate a project to develop lessons using workstations more advanced than the IBM PC or the Apple MacIntosh. Recently, such a project has been initiated at the University of Washington with NSF support. The project will prepare computer programs that produce high-resolution, two- and three-dimensional graphical output. Programs will be prepared for the simulation of chemical



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Warren D. Scider is Professor of Chemical Engineering at the University of Pennsylvania. He served as the first Chairman of CACHE and has been Chairman of the Curriculum Task Force since 1984. Warren is a coauthor of Flowtran Simulation—An Introduction. His research interests are in process analysis, simulation, design, and control. He received his B.S. degree from the Polytechnic Institute of Brooklyn and his Ph.D. from the University of Michigan. He was elected a director of the AIChE in 1983.

reactions, fluid flow, and heat and mass transfer. The reactor design programs will calculate temperature and composition profiles when axial and radial dispersion are important and when mass transfer resistance occurs between the bulk phase and the catalyst particles. The fluid flow programs will permit the graphical input of a finite element mesh, the solution of the Navier-Stokes equations, and the display of streamlines, stress lines, vorticity, etc., in two- and threedimensions. The programs should enable the student to better appreciate the interaction between fluid flow, heat and mass transfer, and chemical reaction in the design of chemical reactors.

Courseware Delivery Systems

With the development of the IBM PC lessons and the software being generated at the University of Michigan and the University of Washington, the Curriculum Task Force will be considering the adoption of a courseware delivery system. One such system, which was created under the direction of Prof. Brice Carnahan (Michigan), is the MICRO-MENTOR system, which is an upgraded version of the MICROCACHE system. MICRO-MENTOR has a more complete data structure for keeping records in large, multi-section courses, an improved format for the preparation of tutorial materials (including text, questions, and followup actions), and permits the intermixing of graphics and text displays.

MICROCACHE, which was developed cooperatively between the University of Michigan and CACHE, with some NSF support, was not considered to be competitive with UNISON for the preparation of frames involving animation and graphics. It was distributed to several universities with modules for completing the material balance of flowsheets with recycle, for binary distillation (using the McCabe-Thiele analysis), and for simple numerical analysis. Eventually, its successor, MICRO-MENTOR, should be reevaluated to determine its utility for the delivery of courseware, both existing and currently being prepared.

Future Directions

What should be the future directions of the Curriculum Task Force? Should it try to define and maintain a model curriculum? To what extent should qualitative reasoning play a role in the preparation of its computer lessons? It seems clear that the logic in creating models for fluid flow, heat and mass transfer, and chemical reaction, can be automated in computer modules that help the student to learn the basic principles. Time will tell to what extent artificial intelligence and expert systems will play a role. Much will also depend on the extent to which statistical mechanics and molecular dynamics impact undergraduate cousework. With faster workstations, equipped with vector processors, and high-resolution displays, statistical methods may gain importance in teaching the concepts of thermodynamics and reaction kinetics.

Whatever the future directions, it seems clear that a strong Curriculum Task Force is a necessary focal point for CACHE. Let us have your suggestions and contributions. The next project of the Curriculum Task Force remains to be defined. If you would like to participate, please contact: Warren Seider (215-898-7953; FAX - 215-898-1130, E.Mail: SEIDER@CHEME.SEAS.UPENN.EDU - (an

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James O. Wilkes has been a chemical engineering faculty member at the University of Michigan since 1963. He was a student and faculty member at the University of Cambridge for eight years before coming to the U.S.A. in 1960. He received his Ph.D. from Michigan in 1963. He has recently been appointed as an Arthur F. Thurnau Professor and Assistant Dean of the College of Engineering at the University of Michigan. His professional interests are in numerical methods, fluid mechanics, and undergraduate education. He holds two diplomas in classical organ performance and frequently goes hiking in the American southwest.

Table 1

CACHE Recommendations for Computing in the Undergraduate Chemical Engineering Curriculum. These recommendations appear in *Evaluating Programs in Chemical Engineering*, published by the AIChE Education and Accreditation Committee.

- (a) The engineering graduate should appreciate that a computer program is a formal medium to express ideas about methodology, the control of which is the essential feature in computer programming.
- (b) The engineering student should be familiar with at least one operating system for personal or main frame computers, and with at least one scientific programming language. Familiarity with an operating system implies competence in file manipulation, text editing, graphic display, etc. Competence in a language implies the ability to write programs and sufficient understanding to test and adapt programs written by others.
- (c) The engineering graduate should have experience in the computer-aided acquisition and processing of information; for example, information retrieval from electronic databases and its manipulation, word processing and graphic programs to generate reports, electronic mail, real-time data for operations management, analysis of experimental data, etc.

- (d) Engineering graduates should have experience in the solution of algebraic and differential equations. They should understand the principles of numerical methods and the concepts of convergence and stability.
- (e) Engineering graduates should gain familiarity with the generation of graphic output and the use of spreadsheet programs.

The basic skills defined here can be achieved best if computing technology is integrated throughout the curriculum. Students should be required to write short programs of their own and use programs supplied by others. It is important that students have experience in evaluating programs supplied by others as well as their use.

For scientific computations, additional skills are strongly suggested. Engineering graduates should have:

- (a)experience maximization/minimization (b)exposure to data analysis using statistical calculations
- (c)familiarity with non-numeric programming.

Table 2

CACHE IBM PC Lessons for Chemical Engineering Courses Other Than Design and Control.

Lesson (Program)	Authors	Applicable for Courses in
Slurry Flow in Channels G. Dow and M.M. Denn, Berkeley	B. Freeman, W. Provine	Fluid Mechanics
Supercritical Fluid Extraction	J.Kellow, M.L. Cygnarowicz and W.D. Seider	Separations and Thermodynamics
Gas Absorption with Chemical Reaction	K. Nordstrom and J.H. Seinfeld, Cal. Tech.	Separations
Design of Flash Vessels and Distillation Towers	B.A. Finlayson, E.W. Kaler, and W.J.Heideger, Washington	Separations and Thermodynamics
Heterogeneous Reaction Kinetics	J.E. Bauer and H.S. Fogler, Michigan	Reactor Analysis
CSTR Dynamics and Stability	L.E. Vajdi and D.T. Allen, UCLA	Reactor Analysis

Table 3

IBM PC and PS/2 Lessons for the Fluid Mechanics Course.

Lesson (Program)

Authors

MACROSCOPIC ANALYSIS:

Pipe Flow

D. Karman, N. Brunswick

Conservation of mass, momentum, and energy is demonstrated graphically for a conduit with typical elements (pumps, pipes, venturi meters, packed beds, valves, etc.) The student can explore various configurations and parametric variations.

Optimal Design of a Pump and Piping Network

J.O. Wilkes, Michigan

The continuity and momentum balances in the steady state are solved to analyze alternative designs for the expansion of a residential piping network. The lesson introduces the synthesis of alternative designs and fault diagnosis.

MICROSCOPIC ANALYSIS:

Stress and Deformation: Couette and Squeezing Flow Between Parallel Plates

K. Ellwood and T. Papanastasiou, Michigan

Couette flow between parallel plates that create shear stresses and shear deformation is displayed by tracing control volumes of material squares as they flow and deform, driven by a moving boundary or alternatively by a pressure difference. Squeezing flow creates normal stresses and deformation, which are also displayed for the appropriate deformable control volumes.

Problems that Require Differential Balances

M.J. McCready, Notre Dame

The lesson leads the student through the formulation and solution of differential systems for flows in common geometries (tubes, annuli, and flat plates) caused by gravity, pressure gradients, and moving boundaries, and involving Newtonian and non-Newtonian fluids.

Fluid Identification

S. Bike, D. Kappler, and S. Maser, Michigan

Given a fluid with unknown rheological characteristics, the student identifies the fluid type (i.e., Newtonian, shear-thinning, etc.) through simulated experimental tests with the cone-and-plate and coaxial cylinder viscometers. Working with the constraint of available volume of fluid for testing, the student must select not only the operating parameters for the viscometers, but also the correct graphical representation of the data for regression.

A User's Guide to Electronic Mail (Part 2)*

Peter R. Rony, Virginia Tech

(*continued from the Fall '89 issue of CACHE News)

UUCP/USENET

The UNIX to UNIX CoPy network (UUCP) includes of order 7000 hosts, most running the UNIX operating system. The network mostly uses simple dial-up modem connections, with TCP/IP network connections where possible. The first links were made in 1978 at Bell Laboratories. Each host pays for its own links, which are generally low-speed (1200 and 2400 baud) and low-cost. Administration is minimal. Typical delivery times are on the order of days. UUCP host-names are non-hierarchical. Some examples are aardvark, edison, groucho, kludge, tukey, yoyo, and zyx. The UUCP network is unusual in using explicit source-routing, in which addresses of the form hosta!hostb!host!user are interpreted as a route along which the message must be sent in order to reach user at host. A few central hosts are known, reasonably reliable forwarding machines; use of these hosts in UUCP addresses makes the Some example routing information shorter. addresses are ...mcvax!ukc!<R>qmc-ms!user (Queen Mary College, London), :cfa,ihnp4,seismo:!noao!sunspot!user (National Solar Observatory, New Mexico). The curly brackets indicate that any of the specified backbone sites may precede !noao!sunspot. The ellipses should be replaced by whatever routing information is needed (if any) to get the message as far as the host name which follow them. The trick in making successful use of UUCP is to be able to determine a routing path from your machine to another machine (as if you had to tell Ma Bell or MCI how to route your phone calls!). Some sites have software that can provide routing information; if you cannot provide the full route, the program will try to determine a route for you automatically. There are a number of UUCPrelated networks: EUNET in Europe (900 hosts), JUNET in Japan (160 hosts) and ACSNET in Australia (see Section 2.7). In Europe, there is one backbone site in each country, e.g., TUT in Finland, INRIA in France, ARIADNE in Greece, MCVAX in the Netherlands, ENEA in Sweden, and UKC in the United Kingdom. All the European backbone sites are connected to MCVAX in Amsterdam, which also connects to SEISMO, the main routing node in the USA. Examples of other backbone sites are MUNNARI in Australia (Melbourne) and UUNET in the United States. From the INTERNET mail can be relayed through uunet.uu.net.

For more information about UUCP send a message to info-server@sh.cs.net with the text:

request: info topic: usenet map topic: ml-3

GTE Telenet

Telenet is a commercial network with a mail service run by GTE. A number of scientists are on this network, particularly the oceanographers and the VLBI crustal dynamics community. NASA uses Telenet systems to provide services for its NASAMAIL and GSFCMAIL networks. Telenet has a large number of local telephone numbers and with a modem and a PC a user can connect to the network from nearly anywhere in the United States. Users are not dependent upon their institutions being wired up to one of the major networks. Telenet charges a fee based on the connect hours used.

Telenet addresses are of the form [username/site]<R>network/country. The four most active Telenet networks for astronomers are TELEMAIL (physicists), MAIL (some specific institutional networks), NASAMAIL (NASA headquarters and most NASA centers, and GSFCMAIL (Goddard Space Flight Center).

Most users communicate within their own network and do not use the brackets and network/country designations. Within one Telenet network, the username is sufficient if the name is unique. For example, if you are on TELEMAIL and want to send mail to Peter Boyce. then PBOYCE is an adequate address. If you are on NASAMAIL you would have to use the address [pboyce/amerphys]telemail. Conversely, to get to a NASAMAIL user the address would be of the form username/nasa]nasamail. If you stay within the United States, the country designation is not needed. If you have trouble contacting people who say they are on TELEMAIL, try addings the network designation.

The American Institute of Physics is

upgrading an electronic network service is has established called PINET. In addition to listings of jobs, abstracts in advance of publication, meeting notices and other data, it has established an electronic mail service, called PIMAIL, with direct connections to Bitnet and the Internet. PIMAIL subscribers can mail to these networks without having to use gateways. AIP will charge only for the communications costs. Note that AIP will not serve as a gateway between networks, but will allow their subscribers who come in on Telenet to communicate directly and easily with the other two networks. To get more information on PINET contact the PINET Administrator, American Institute of Physics, 335 East 45th Street, New York, NY 10017 (tel. 212-661-9404) or see the ads in Physics Today. To get information on local Telenet phone numbers in your area, call 1-800-336-0437. There are several relays between Telenet and INTERNET, one run by NASA Ames Research Center (POSTMAN), and another run by ISI Intermail.

PSI/DTE International Data Communications

Most countries have public data communications networks that allow national and international calls to be made in support of electronic mail, file transfers, and remote logins. To make a call to a remote computer, is necessary only to know the machine's DTE (Date Terminal Equipment) number, often quoted as a PSI (Packetnet System Interface) number, DNIC number, or X.25 number.

The X.25 protocols (X.3, X.25, X.28, ..., sometimes known as "Triple-X") may be used directly to establish connections with remote host computers. International gateways (using the X.75 protocol) ensure that links can be made between countries. The Triple-X protocols are used by a number of other networks to provide connections between sites. Most of these X.25 links are not visible to network users, but they do provide many gateway-gateway links in INTERNET, CSNET, and UUNET. Also, these protocols are the underpinnings for the Telenet networks, the new international mail standard X.400, and for DEC's PSI. PSI supports mail, remote logins, and remote file transfers, and there are several relays between PSI mail and other networks.

Each DTE number is unique to a given machine and is internationally recognized. The first 3 digits are a country code, the 4th digit distinguishes individual networks within the country, and the next 8 (or so) digits are used to distinguish physical lines on the network. As well as this total of approximately 12 digits, 3 more digits may be added to specify local subaddresses (individual computers) sharing the given

line. Some countries allow only one digit for the sub-address, others allow two, and a few allow three. DTE numbers are often quoted with a zero preceding the country code. The DTE number functions much more like the standard telephone numbers we are accustomed to; the DTE address is the same regardless of your particular host.

Since DTE numbers are generally long, difficult to remember, and easy to mistype, some sites will set up alias tables for commonly addressed sites. These allow users to refer to the site by a simple name rather than by the DTE number.

On DEC systems you may see addresses of the form PSI%HOST or PSI%31103010014012, the latter being the DTE number.

The names of the data communications are different countries and their international DTE codes are listed in Table 2.

Other Networks

ASCNET. The Australian Computer Science Network includes over 300 hosts (1986) and caters to a mix of academic and commercial clients. The network is UNIX-based and began operating in 1979. Each host pays for its own links. The naming syntax, like that of the Internet, is hierarchical. An example of a host-name on ACSNET is suphys.su.oz.au (Physics Department, Sydney).

For information contact postmaster@munnari.oz.au, or ACSNET Coordinator, Department of Computer Science, University of Sydney, New South Wales 2006, Australia.

CDNNET. The Canadian Universities' X.400 network includes approximately 65 hosts. An example of a host-name on CDNNET is drao.nrc.cdn (Dominion Radio Astrophysical Observatory). For information about CDNNET contact CDNNET HQ, Computer Centre, University of British Columbia, Vancouver, British Columbia V6T RWS, Canada.

Canada is now involved with a major network project called NRCNET which is to provide high speed, full function network links across Canada. In February 1989, the CSNET board and trustees approved the merger of CSNET and BITNET. For information about this initiative, contact woodsworth@nrcdao.<R>bitnet.

CSNET. The Computer Science Network includes many hosts in the USA and at international sites. Host names are hierarchical. An example of a host-name on CSNET isandy.bgsu.csnet, a machine at Bowling Green State University. CSNET only offers mail

services but uses a number of different network links. CSNET also runs an information server and a relay system that can be reached from INTERNET relay.cs.net. For information on CSNET, send a message containing the following lines to info-server@sh.cs.net:

request: info topic: help request: end

HEPNET. The High Energy Physics network includes over 600 hosts, 150 of them in Europe. An example of a host-name on HEPNET is MINN (node 43077), at the University of Minnesota. HEPNET uses both DECNET and Coloured Book protocols. The DECNET addresses are coordinated with SPAN.

INFNET/ASTRONET. The Italian research network uses the DECnet protocols and includes approximately 100 hosts. ASTRONET is a subset of INFNET consisting of nodes at major Italian astronomy research centers.

INFNET hosts can be reached via the BITNET/EARN gateway CERNVAX at CERN, Switzerland, and are also accessible on the SPAN network. For example, the INFNET host astbol, serving the Radio Astronomy group in Bologna, is also SPAN host astbol, node number 39.126 (40062). EARN addresses for INFNET users are sometimes quoted as user@host.bitnet. For more information about INFNET/ASTRONET contact astrts::adoc.labeljanet.

JANET. The UK Joint Academic (X.25) Network includes approximately 1000 hosts. All UK universities and most polytechnics and connected. The network originated with SERCNET (the Science and Engineering Council Network) in 1977, and was renamed JANET in 1984. The cost of leasing lines from British Telecom is met through grants from the SERC. Electronic mail and other services are implemented using the UK Coloured Book protocols. Each Coloured Book defines a different standard. For example, the Grey Book defines a temporary network mail protocol based on the RFC733 header standard (following an ARPA INTERNET convention.)

Host names conform to a National Registration Scheme (NRS), managed by Salford University, and are hierarchical like those of hosts on the Internet, but with the most significant element first. For example, uk.ac.ucl.cs.ness is the INTERNET gateway at University College, London, and uk.ac.umrcc is the Manchester Computer Centre.

AC stands for Academic Community, i.e., it corresponds to the EDU part of the Internet.

There is also a CO domain catering to commercial clients.

Within JANET the uk.ac may be omitted. There are also standard abbreviations for some names, e.g., rgo.star for ro-greenwich.starlink. For JANET NEWS, login to uk.ac.janet.news (userid news). For more information contact Network Executive, Rutherford Appleton Laboratories, Chilton, Didcot, Oxon OX11 OQX, United Kingdom.

SolarMail. SolarMail is an electronic mail distribution system run by Rick Bogart of Stanford University for solar astronomers. With mailboxes on SPAN, INTERNET, and BITNET, this can be a convenient way to contact solar astronomers or receive notices of interest to the solar community. For further information contact rick@solar or solar::rick.

Starlink. The UK astronomers' DECnet-based Starlink network (9300/19200 baud lines) is funded by the Science and Engineering Research Council and includes 10 VAX hosts. There are associated Microvaxes at several other British universities.

3. Hints on Deciphering Electronic Mail Addresses

To the novice, many electronic mail addresses appear to be incomprehensible jungles of acronyms and punctuation marks. Below are a few hints on deciphering them, followed by some real-life examples.

*All the alphabetic and numeric characters, including @ %! - ":., may appear in electronic mail addresses. Percent signs (! signs for UUCP) usually separate the names of hosts through which the message is to be routed. For example, a message to user%host%host1%host2@host3 will be sent to host3, which will in turn forward the message to user%host%host1 at host2, and so on. Exclamation marks, curly brackets, and ellipses are used in specifying UUCP addresses. Colons are used in DECnet addresses to separate the host name form the user name and in some INTERNET addresses.

*To determine the network of origin, look at the form of the sender's address in the 'from' field in the header. An address of the form user@host or user@host.domain has probably originated on INTERNET or BITNET/EARN. UUCP addresseswill be punctuated by exclamation marks (host1!host2!host3!user). Addresses on SPAN (and other DECNET based networks, such as INFNET and Starlink) have a host name and user

name separated by two colons (host::user).

*Host names on INTERNET, ACSNET, CSNET, and JANET are hierarchical, of the form domain1.domain2.domain3. Most networks with hierarchical naming place the least significant domain (i.e., the final destination machine) first (host.site.domain). In JANET addresses the most significant domain comes first, e.g., uk.ac.rogreenwich.starlink, and JANET names must often be reversed when communicating with networks outside the UK. Hence, for example, starlink.rogreenwich.ac.uk is the address quoted by RGO to BITNET users. Note that the elements neighboring the hyphen retain their original order i.e., the hyphen is treated like an alphabetic character that is part of the domain name.

*Internet names frequently end in .edu, c.g., noao.arizona.edu. Less common (to astronomers) will be addresses from the domains .com, .gov, .mil, and .org.

* SPAN and other DECNET (INFNET/ASTRONET, HEPNET, Starlink) hosts are sometimes referred to by area and number or by number alone. You may have to use the numerical address if the node names are not present in your local site table.

The most general form of an address where the message must pass from one network to another, or through some intermediate host, has the form user%host.domain@relay.my domain.

The message is sent first to the computer called relay which is in a network my_domain that your local system can reach. The computer relay then passes the message on to the remote machine called host in the network domain. The computer relay may actually modify the address you specify in order to perform the message forwarding. In cases where the remote address is of some peculiar form, or where the relay host does not know how to modify it, the remote part of the address will generally get written inside quotation marks. For example,

"astrts::adoc"@io.arc.nasa.gov

will relay a message from INTERNET (note the .gov domain) to the user adoc at the ASTRONET site astrts.

4. Sending Electronic Mail Across Networks

Mail crosses network boundaries through forwarding systems known as gateways or relays. It is often necessary to find a route to a user that utilizes one of these gateways. Table I can be used to find routing information from on network to another. For example, a user on BITNET could send mail to a user on SPAN by making use of the gateway at SDSC:

user%host.span@sdsc.bitnet

or a use on INTERNET could send mail to a BITNET user using the gateway at CUNYVM:

user%host.bitnet@cunyvm.cuny.edu

This table can also be used to work out return addresses. As shown in the table, many combinations are possible and there may be one or more relay systems that serve the same networks. The table lists possibly redundant relays because individual relays may be down at times and because relays may cease service.

Much of the information in the table is taken from Quarterman and Hoskins (1986). The syntax for messages is traveling to and from SPAN were provided by the SPAN Network Information Center at NSSDCA (dated September 1987). Dates indicate the last time a particular syntax was tried and found to work. Confirmation of others would be appreciated.

In the UK hierarchical host-names must be entered in reverse order. In the table the context makes clear the order required. For example, JANET names may need to be specified as uk.host or host.uk. Note that while most gateways support open access, authorization may be required in order to use some gateways. For example, UK users must register in order to use the gateways at uk.ac.ucl.cs.nss (INTERNET), uk.ac.rl.earn (BITNET/EARN) and uk.ac.ukc. (UUCP). Limits are also imposed on the lengths of records and sizes of files (typically a few tens of kbytes) that may be mailed through gateways. Binary files will not usually transmit in the form of mail over networks, although programs are available for converting some kinds of binary data to ASCII data.

Relays through which a message passes have mailers for forwarding the message according to the address it bears. If one of the hosts is down the message may be sent via another route, returned to the sender, delayed, or lost. The rcply, if it comes at all, may do so by a quite different route. For example, replies to JANET addresses sometime attempt to enter the United Kingdom by the

Internet gateway, and messages directed at it are frequently bounced. Most UK users are authorized to use the EARN gateway.

Most mailers at gateways require the message to be in a Batch Simple Mail Transfer Protocol envelope. Many BITNET users are on campus networks and can be reached only by sending mail to the mailer at the gateway for that campus. Many BITNET hosts have programs that simplify the task of sending mail from BITNET to other networks by supplying the BSMTP envelope when needed and sending the mail to the correct mailer and gateway. These programs are usually SENDGATE for IBM/VM systems, and GMAIL or PMDF for DEC VAX/VMS systems. Such a program can only send mail to domains it knows the gateways for, and unfortunately, the files of mailers and gateways used by these programs are sometimes incomplete. For example, the July 1989 version of DOMAIN NAMES from listserv@bitnic does not list the oz or oz.au domains, but the equivalent files, BITNET GATES, does. On the other hand, DOMAIN NAMES contains some entries that are not in BITNET GATES.

If you know a host address but not the individual user's address, try using the surname, first initial plus surname, or the user's initials. Some sites have alias tables set up for their staff so that mail arriving at any of a number of names will be forwarded to (hopefully) the right person. You can also try sending mail to postmaster (recommended), root (for UUCP), system (will probably work), or oper (last resort), and specify the name of the recipient in the first line of text. Since systems managers and computer operators will generally not care to continue handling your misguided mail, they may well provide you with a proper address for the intended recipient. Postmasters tend to be user friendly sorts who are willing to help the mail get to its final destination.

Because of the possibility that an outgoing message may disappear down a black hole, it is recommended that user's append to each message (a) a request for confirmation, and (b) their network and postal addresses and their telephone and telex numbers. All of this is not necessary once you have exercised a particular e-mail routing a few times and have some confidence that the mail will get through. Hopefully, in time, the current complexities of electronic mail will disappear and something like the relative simplicity of the national and international telephone systems will replace it. In the meantime, patience, this guide, and the help of a local e-mail "guru" will help a lot.

Glossary

ACSNET Australian Computer Science

Network

ADONIS proposed Eastern Bloc network,

see New Scientist 17/9/87

AGRINET UK agricultural research

DECnet

Ames NASA Ames Research Center,

Sunnyvale, California

ARPA Advanced Research Project

Agency network

ASCII American Standard Code for

Information Interchange

(character set)

ASTRONET part of INFNET

AUSEANET microelectronics network, S.E.

Asia and Australia

baud maximum number of changes of

state per second; usually =

bits/second

BITNET "Because It's Time" Network block area of space on disk, typically

area of space on disk, typically

hundreds bytes (vendor

dependent)

bps bits per second

byte 8 bits (a character usually

occupies one byte)

CCITT International Consultation

Committee on Telegraphy and

Telephony

CCSDS Consultation Committee on

Space Data Systems Canadian network

CDNNET Canadian networ CERN, CHUNET Swiss EANs

Coloured Book a set of standards that attempts

to conform to the ISO ideal; each is written up as a different

coloured book

COM ARPA Internet network for

commercial clients

COSAC French research network

(<F129M> 27 hosts)

CSNET Computer Science Network

CYPRESS part of CSNET

DDN Defense Data Network =

ARPANET + MILNET+

MINET+ DISNET

DEC Digital Equipment Corporation

DECnet proprietary networking

protocols developed by DEC for

PDP11, VAX

DFN German EAN Deutsche

Forshungnetz, W. Germany

DISNET part of DDN

DRENET ARPANET-like Canadian

military network

DTE	Data Terminal Equipment	NL	Dutch EAN
EAN	number X.400 networks in Australia,	NORDUNET NORTHNET	Nordic network Canadian BITNET
EARN	Canada, Europe European Academic Research	NRS	Name Registration Scheme (for JANET)
EBCDIC	Network Extended Binary Coded Decimal	NSFNET NSSDC	part of CSNET National Space Science Data
EDU	Interchange Character set (IBM) ARPA Internet network for	OSIRIDE	Center at GSFC Italian EAN
ESANET	academic/research clients European Space Agency Network	packet	typically between 1 and 255 bytes
ESPIN	European Space Information (part of SPAN)	packet switching	use of a communications channel
Ethernet	local area network defined by ISO 802,3	· ·	by multiple users whose data are split <r> into individually</r>
EUNET	European affiliate of UUCP		identified packets
Fax	facsimile transmission	PACNET	Pacific hosts network
FIDONET	cooperative network in United States (1000 hosts)	PAD	Packet Assembler/Disassembler, interfaces host with X.25
FNET	French UUCP network, part of EUNET	PSI	network Packetnet System Interface
FTAM	File Transfer and Management		(VAX/VMS)
ETD	(ISO file transfer)	PSN	Packet Switched Node
FTP	File Transfer Protocol (part of	PSS	Packet Switched Service
antarros.	ARPA file transfer protocols)	RARE	ESPRIT-funded project to creat
gateway	computer providing message transfer service between		European meta-network
	networks	relay	computer providing message
GSFC	Goddard Space Flight Center,		transfer and translation services
OOLC	Greenbelt, Maryland	ROSE	between dissimilar networks
GSFCMAIL	Telenet-based mail network for	KOSE	ESPRIT-funded project; Research Open Systems for
ODI CIMALE	GSFC		Europe Europe
HEPNET	High Energy Physics Network	RSCS	Remote Spooling and
host	computer	RSCS	Connection Subsystem protocol
IMP	Interface Message Processor,		used by BITNET
	used in ARPA	SATNET	ARPA Internet satellite links
INFNET	Italian DECnet	SDN	South Korean cooperative
IP	Internet Protocol, basis of		network (<f128m> 100 hosts)</f128m>
	ARPA protocols	SMTP	Simple Mail Transfer Protocol
IPSS	International PSS		(ARPA)
IRIS	Spanish EAN	SPAN	Space Physics Analysis Network
IRL	Irish EAN	Starlink	UK astronomy DECnet
IS	International Standards Org.	SUNET	Swedish EAN network
JANET	Joint Academic Network (UK)	SURF	Dutch network
JUNET	Japanese UUCP-like research	SWITCH	Swiss network
	network (<f128m> 160 hosts)</f128m>	TCP	Transmission Control Protocol,
KEK	a Japanese network		used by Internet
line speed	data transmission rate	Telemail	Telenet mail services
MAILNET	USA research network (28 hosts) started at M.I.T.	Telenet	commercial network in United States
MFENET	Magnetic Fusion Energy research network, USA	TEXNET TP0 - TP4	DECnet-based network in Texas Transmission Protocols in the
MILNET	USA defense network (part of		ISO suite
MINET	ARPA Internet)	TYMENET	commercial network in the
NASAMAIL	European hosts on MILNET Telenet-based network for	IMINETT	United States
MASAMAIL	NASA employees, contractors,	UNINETT	Norwegian EAN
	and scientists	UNIX	operating system (pun on MULTICS)
NCP	Network Control Protocol		WIGETICS)
	(DECnet)		
	(===000)		

Page 14 Spring 1990

USENET	alternative name for UCCP network	X.29	international standard for terminal calls over X.25
UUCP	Unix to Unix CoPy network		network
VNET	IBM's company network	X.400	new international standard for
X.25	international standard for		electronic mail
	operation of a packet switched	X.500	new international standard for
	network		name and directory services
X.25NET	part of CSNET	XNS	Xerox Network System
			company network<>

Table 1 Network Gateways

From	<u>To</u>	Syntax
ACSNET	ACSNET ARPA BITNET JANET JUNET SPAN UUCP	user@host.OZ.AU user%host.domain@MUNNARI.OZ user%host.BITNET@MUNNARI.OZ user%host.UK@MUNNARI.OZ user%host.JUNET@MUNNARI.OZ user%host.SPAN@VLSI.JPL.NASA.GOV user%host.UUCP@MUNNARI.OZ
BITNET	ACSNET ARPA ARPA BITNET JANET JANET JUNET SPAN UUCP	user%host.OZ.AU@relay user@host.domain user%host.domain@relay user@host user%host.UK (Nov 1987, recommended) user%UK.host@AC.UK (Sep 1987) user%UK.host@UKACRL (Sep 1987) user%host.JUNET@RELAY.CS.NET user%host.SPAN@SDSC.BITNET host1!host2!host!user@PSUVAX1
INTERNET	ACSNET ACSNET ARPA BITNET CSNET JANET JANET JUNET SPAN SPAN SPAN SPAN UUCP	user@host.OZ.AU user%host.OZ@UUNET.UU.NET user%host.domain user%host.BITNET@CUNYVM.CUNY.EDU user%host.CSNET@RELAY.CS.NET user%host.UK@NSS.CS.UCL.AC.UK user%host.UK@IO.ARC.NASA.GOV user%host.JUNET%UTOKYO-RELAY@RELAY.CS.NET user%host.SPAN@NSSDCA.GSFC.NASA.GOV user%host.SPAN@STAR.STANFORD.EDU user%host.SPAN@VLSI.JPL.NASA.GOV user%host.SPAN@IO.ARC.NASA.GOV user%host.SPAN@IO.ARC.NASA.GOV

JANET	ACSNET	backbone-site!host.OZ!user@UK.AC.UKC (Nov 1987)
	ARPA	
		user%domain.host@UK.AC.RL.EARN (Nov.1987)
	ARPA	user%host.domain@UK.AC.UCL.CS.NSS (Nov. 1987)
	BITNET	user%host@UK.AC.RL.EARN (Nov. 1987)
	CDNNET	user%CDN.host@UK.AC.RL.EARN (Nov. 1987)
	CSNET	user%CSNET.host@RL.EARN
	HEPNET	user%CERN.DECNET.host@UK.AC.EAN-RELAY
	HEPNET	user%host.HEPNET%LBL@UK.AC.RL.EARN
	INFNET	
		user%host.INFNET%BITNET.CERNVAX (Nov. 1987)
	INFNET	user%INFNET.host@UK.AC.RL.EARN
	JANET	user@UK.host (Nov. 1987)
	JUNET	user%host.JUNET@UK.AC.UKC
	SPAN	user%host.SPAN%STAR.STANFORD.EDU
		@UK.AC.UCL.CS.NSS (Nov. 1987)
	SPAN	user%host.SPAN%EDU.STANFORD.STAR
		@UK.AC.RL.EARN
	SPAN	user%host.SPAN%VLSI.JPL.NASA.GOV
	DITTI	
	CDAN	@UK.AC.RL.EARN
	SPAN	MAILER%host::user@PSS.ESOC.FTP.MAIL
	SPAN	user%host.SPAN%VLSI.JPL.NASA.GOV
		@UK.AC.UCL.CS.NSS
	UNINETT	user%host.UNINETT@UK.AC.EAN-RELAY (Nov. 1987)
	UNINETT	user%UNINETT.host@UK.AC.RL.EARN (Nov. 1987)
	UNINETT	host.UNINETT!user@UK.AC.UKC
	UUCP	host1!host2!host!uscr@UK.AC.UKC (Nov. 1987)
	UUCP	host1!host2!host!user%UUCP.backbone-site (Nov. 1987)
	0001	nostrinostzinostiuser/000erioaekoone-site (140v. 1987)
JUNET	ACSNET	waar@haat OZ AII
JUNEI		user@host.OZ.AU
	ARPA	user@host.domain.ARPA
	BITNET	user@host.BITNET
	JANET	user@host.UK.JANET
	JUNET	user@host.JUNET
	SPAN	user%host.SPAN@VLSI.JPL.NASA.GOV
	SPAN	KDDLAB!user%host@IO.ARC.NASA.GOV
	UUCP	user@host.UUCP
	ccci	user@ 110st. 0 0 C1
SPAN	ACSNET	NSSDCA::EXOS%"user@domian.OZ.AU"
OI /III		
	ACSNET	JPLLSI::"user@domain.OZ.AU"
	ARPA	NSSDCA::EXOS%"user@host.domain"
	ARPA	STAR::"user@host.domain"
	ARPA	JPLLSI::"user@host.domain"
	ARPA	SDSC::"user@host.domain"
	BITNET	NSSDCA::EXOS%"user%host.BITNET"
	BITNET	HAMLET::"user%host.BITNET"
	BITNET	STAR::"user%host.BITNET"
	BITNET	JPLLSI::"user%host.BITNET"
	BITNET	SDSC::"user@host.BITNET"
	JANET	JPLLSI:: "user%host.domain@NSS.CS.UCL.AC.UK"
	JANET	NSSDCA::EXOS%"user%host
	LANDE	@NSS.CS.UCL.AC.UK"
	JANET	STAR::"user%host@NSS.CS.UCL.AC.UK"
	JUNET	JPLLSI::"user%host.JUNET@RELAY.CS.NET"
į.	JUNET	IO::"!KDDLAB!host!user@RELAY.CS.NET"
	UUCP	IO::"host2!host1!host!user@UUNET.UU.NET"
	UUCP	NSSDCA::EXOS%"host2!host1!host!user
		@UUNET.UU.NET"
	UUCP	JPLLSI::"host2!host1!host!user@UUNET.UU.NET"
	JUCI	JI ELOI HOSE. HOSE HOSE USER WOUNE I. OU. NE I

UUCP	ACSNET	UUNET!MUNNARI!host.OZ.AU!user
	ARPA	UUNET!host.domain!user
	BITNET	PSUVAX1!host.BITNET!user
	JANET	relay!NSS.CS.UCL.AC.UK!host.UK!uscr
	JUNET	relay!host.JUNET!user
	SPAN	user%host.SPAN@VLSI.JPL.NASA.GOV
	SPAN	user%host@IO.ARC.NASA.GOV
	UUCP	host1!host2!host!user

Where the word domain appears in the above table, the name of one of the INTERNET top-level domains, e.g., COM, EDU, should be substituted. Note that all references to the node IO should be replaced by the name AMES.

Table 2 International DTE Communications Access Codes

Country	DTE Code	Date Communications Networks
Austria	2322	DATEX-P
Australia	5052	AUSTPAC, MIDAS
Belgium	2062	DCS
Brazil	7241	RENPAC, INTERDATA
Canada	3020	DATAPAC, GLOBEDAT,
	2020	INFOSWITCH
Denmark	2382	DATAPAK
Finland	2442	DATAPAC
France	2080	TRANSPAC
Germany (West)	2624	DATEX P
Greece	2022	HELPAC
Ireland	2724	EIRPAC
Israel	4251	ISRANET
Italy	2222	ITAPAC
Japan	4401	DDX P, VENUS P
Netherlands	2041	DATANET1, DABAS
New Zealand	5301	PACNET
Norway	2422	DATAPAK
Portugal	2680	(incoming only)
South Africa	6550	SAPONET
Spain	2145	IBERPAC, TIDA
Sweden	2405	DATAPAK
Switzerland	2284	TELEPAC
United Kingdom	2342	PSS
United States	3126	AUTONET
	3132	COMPUSERVE (outgoing only)
	3103	ITT-UDTS
	3113	RCA-LSDS
	3110	TELENET
	3119	TRT-DATAPAC
	3140	SNET
	3106	TYMENET
	3125	UNINET
		WUI-DBS
	3101	WUTCO

Partitioning of Pollutants in the Multimedia Environment: The SMCM Software

By Yoram Cohen, Wangteng Tsai and Steve Chetty University of California, Los Angeles

Abstract

This paper describes the spatial-multimediacompartmental (SMCM) software package designed for the study of the partitioning of pollutants in the multimedia environment. The SMCM software was developed specifically for the Chemical Engineering undergraduate program, and it can be used for illustrating principles of transport phenomena, phase equilibria, and mass conservation. The SMCM software has also served as a research tool and it has been used in conjunction with exposure and risk analyses in a senior undergraduate elective/first level graduate course on pollution control. The main features of the SMCM software are described in this paper. and selected examples of the scenarios that can be simulated are discussed.

Introduction

Chemical engineers have the obligation to work towards pollution prevention. Therefore, they must be educated to understand the potential problems that can occur due to environmental contamination. In order to evaluate the potential risk due to the release of various chemicals to the environment one must be able to forecast their probable concentrations in the environment, the exposure of human and ecological receptors to those chemicals, and the associated health and ecological risks [1]. One must realize first that the distribution of pollutants that are released to the environment among the various environmental compartments is the result of complex, physical, chemical, and biological processes. Furthermore, the potential hazards of various pollutants released to the environment depend upon the degree of multimedia exposure of human and ecological receptors to these chemicals and the associated risks.

Given the high cost of environmental monitoring, the prediction of pollutant concentrations in the multimedia environment via appropriate fate and transport models is essential for appropriate exposure and risk analyses. Chemical engineers, with their strong background in transport phenomena, phase equilibria, and reaction engineering, possess all the basic

ingredients that are required to tackle the above problem. The problem of predicting the multimedia partitioning of pollutants in the environment is obviously a complex task. Nonetheless, it is possible to construct relatively simple yet practical models that can allow the chemical engineering practitioner and student to explore the ideas that encompass the subject area of pollutant partitioning in the multimedia environment. Through such a study, for example, the chemical engineering student can gain an appreciation for the applications of transport phenomena and thermodynamics to the "real world". The key instructional challenge has been to allow the student to investigate the above subject area in a reasonable time period of 3-5 weeks. This task has been made possible with the introduction of an IBM PC simulation tool as described below.

In order to provide a convenient and accurate simulation tool for the environmental multimedia partitioning of pollutants, the userfriendly Spatial Multimedia Compartmental (SMCM) model was developed at UCLA through the sponsorship of the UCLA/EPA National Center for Intermedia Transport Research (NCITR). The SMCM software is a tested research tool that has been utilized by the NCITR over the last five years. The SMCM model is well suited for those users who are interested in getting a better understanding of pollutant distribution in the environment and prefer not to spend the time to learn complicated programing skills or the complex operational procedures required with most environmental software.

Configuration and Features of the SMCM Software

The SMCM is a screening level IBM PC based model designed to estimate the multimedia partitioning of organic pollutants in local environments. The model makes use of both uniform (well mixed) and nonuniform (one-dimensional) compartments. The configuration of the SMCM model is shown in Figure 1. The

Table 1 Features of the SMCM Model

1. The SCSM is a user-friendly software package that:

- a. Can be used to answer "what if" type questions.
- b. Allows for rapid scenario changes.
- c. Minimizes data input.
- d. Provides a graphical output display for quick scenario analysis.
- e. Provides specific online help for input data fields.
- f. Provides a menu system for user selection of data input, simulation execution, plotting, and printing a summary report of the calculated results.
- g. Allows the software to be run on IBM-PC/XT/AT compatible computers.
- h. Allows an inexperienced user to run the SMCM software with virtually no ackground in transport phenomena.

2. The SMCM model applies a new modeling approach that:

- a. Makes use of both uniform (air, water, biota, suspended solid) and non-uniform compartments (soil and sediment).
- b. Allows for mass exchange of pollutant between the air compartment and its surrounding atmospheric environmnet. The water compartment is also treated in a similar way.
- c. Treats non-uniform compartments as an unsteady state, one-dimensional diffusion type equation with convection and chemical reaction.
- d. Incorporates the simulation of a chemical buried in the soil compartment.
- e. Considers a variety of source types and allows the user to select and input source date through the data input screens.
- f. Applies flux boundary conditions for non-uniform compartments. Although groundwater is not trested as a compartment in the SMCM model, flux condition at the bottom boundary of the soil compartment can be incorporated to account for the chemical transport to groundwater.

3. The SMCM model accounts for the effects of rainfall and temperature on the environmental transport of pollutants:

- a. The SMCM has a rain generation module which can generate rainfall in the form of a single event of specified intensity and duration, or randomly distribute rainfall within specified levels of rainfall intensity, duration and total rainfall.
- b. The transport processes associated with rainfall such as rain scavenging, infiltration, runoff, and soil drying are simulated by a water balance method which uses theoretically based correlations.
- c. User-supplied average monthly temperatures are used to construct average daily temperatures.

4. Provides accurate and reliable parameter estimation methods:

- a. Physicochemical parameters such as mass transfer coefficient, diffusion coefficient, and partition coefficient are estimated using theoretical methods and empirical correlations. The user can input partition coefficients and diffusion coefficients if known. These will override any model-estimated values.
- b. Temperature variations of diffusivities, partition coefficients, mass transfer coefficients, and reaction rate constants are included by either internal predictions or via user-input data.
- c. Production or degradation rates are treated as first order reactions.

model consists of coupled partial and ordinary differential equations that are solved simultaneously by a finite difference method and using the operator splitting technique [2]. The hybrid approach as implemented in the SMCM model is more accurate compared to other existing multimedia models which assume all compartments to be uniform [3]. The SMCM has the capacity of simulating a variety of pollutant transport phenomena as listed in Table 1. Furthermore, accurate parameter estimation methods using theoretical equations and empirical correlations are incorporated in the model such that the user is only required to input basic physicochemical parameters (solubility, molal volume, boiling temperature, molecular weight), compartmental configurations (dimensions), and modest amount of meteorological data (average monthly temperature and precipitation). addition, the SMCM has a module developed specifically for the generation of rain events.

Main Menu and Flow Diagram of the SMCM Software

The SMCM software has a user-friendly interface and is totally driven by a menu system as illustrated in Figure 2. The menu choices include: full screen data input, simulation execution, interactive graphical output, on-screen review of numerical results, print-out of numerical results, and exit to DOS. At any point within the SMCM model, the menu is accessible by pressing a function key as indicated on the screen. A logical

sequence for a complete scenario simulation would be: (1) full screen data input; (2) simulation execution; (3) interactive graphic outputs; (4) review of numerical results; and (5) printing of numerical results.

A schematic description of the structure of the SMCM model is displayed in Figure 3. The data input screens are accessible by pressing selection 1 from the internal menu. The online help facility which accompanies the data input screens for answering implementation questions and providing brief descriptions of required data is available by pressing the {F1} function key. For example. Figure 4 is one of the input screens for air and water compartments, and Figure 5 is the associated online help screen. Once data are entered, the simulation execution is chosen from the main menu. Upon successful execution of the SMCM numerical code, two interactive graphical displays of the results are available by pressing selection 2 (interactive graphics output) from the external main menu. The first plot displays the pollutant concentration versus time for each compartment. The second figure displays a partial plot of pollutant concentration profiles in only three of the compartments in order to provide a clear view of the results. The numerical results can also be reviewed on the screen by pressing selection 3 from the external main menu. Finally, printing of these numerical results can be accomplished by pressing selection 4 from the external main menu. The numerical results are automatically saved in ASCII files and include the concentration profiles in the sediment and soil compartments.

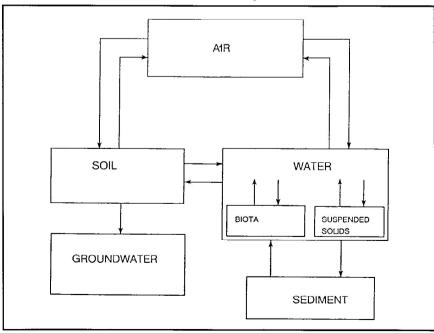


Figure 1 - Configuration of the SMCM model

Page 20 Spring 1990

Possible Simulation Scenarios

In order to provide for a variety of scenario simulations, two types of simulations are provided in the SMCM software. The first is for uniformly distributed (UD) sources and the second is for a buried chemical. Both the UD source and the buried chemical scenario simulations can be run in conjunction with a rainfall simulation. These simulations are briefly described below.

Uniformly Distributed Source Simulation

Four types of uniformly distributed (UD) sources (non-repetitious constant, non-repetitious sinusoidal, constant repetitious, and sinusoidal repetitious) are considered for the air and water compartments, whereas only a non-repetitious constant UD source can be applied for the soil and sediment compartments (Figure 6). The nonrepetitious constant UD source is applicable for scenarios where the pollutant is released with a constant source strength. The source strength is allowed to be turned on and off at times selected by the user. The non-repetitious sinusoidal source case can be applied for scenarios where chemical emission follows the pattern of sinusoidal variation such as chemicals emitted from industrial plumes. In such a case, the SMCM application is appropriate if multiple point sources exist over an area of sufficient size to treat the collection point sources as distributed sources. The constant repetitious source allows the source strength to be turned on and turned off sequentially. Finally, the sinusoidal repetitious source provides for modeling of diurnal or seasonal source variation such as the emissions of pollutants from automobile traffic. In this case, the average source strength may represent the average daily emission rate of the pollutant, whereas the source amplitude represents the maximum (or minimum) variation from the average source strength.

The SMCM model can also be used to simulate the response of an initially polluted system to the elimination of pollutant sources. For such scenarios, sufficiently high initial concentrations (above background) are required as input for the appropriate SMCM compartments.

Buried Chemical Simulation

The second type of simulation which is supported by the SMCM model is the buried chemical simulation. In this simulation, a given mass of a pollutant is buried at an assigned depth, and it is allowed to diffuse both downward and upward through the soil compartment. Upward diffusion will eventually lead to air phase release and distribution among the various compartments.

Case Study: Benzene in the Santa Clara Valley

As an illustration of the SMCM software, a simple simulation of the dynamic distribution of benzene (with a repetitious sinusoidal source in the atmosphere) in the Santa Clara Valley, California is presented. It is noted that before applying the SMCM software to assess themultimedia partitioning of chemicals in the environment for a particular region, one must first gather the required data for the simulation such as the compartment data (e.g. interfacial areas, source types and strengths, soil types), meteorological conditions (e.g. wind speed, monthly mean temperature, precipitation), and physicochemical properties of pollutants. The detailed description

Figure 2. Main menu of the SMCM software

SMCM (VERSION 3.0) INTERNAL MAIN MENU

1. Full screen data input
2. Simulation execution
3. Go to External Menu
4. Exit to DOS

SMCM (VERSION 3.0) EXTERNAL MAIN MENU

1. Full screen data input
2. Interactive graphics output
3. Review numerical results
4. Print numerical results
5. Exit to DOS

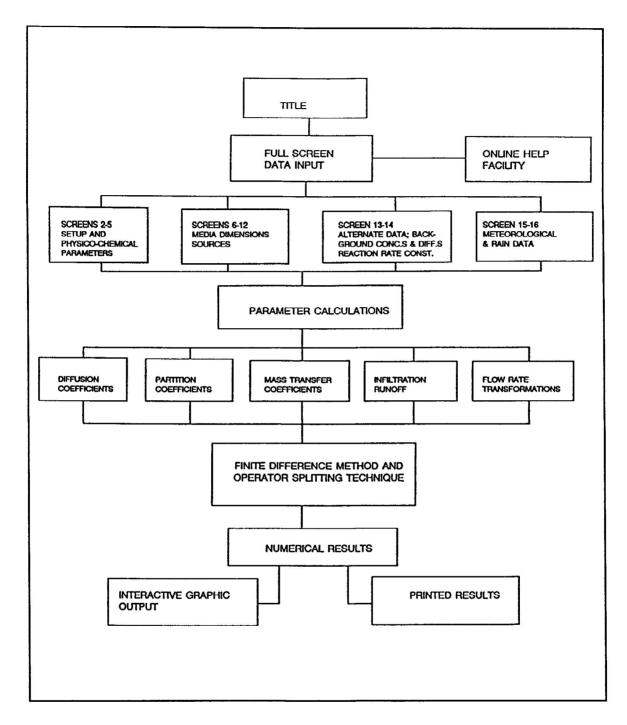


Figure 3 - Flow diagram of the SMCM software

Page 22 Spring 1990

of the required data for the simulation of multimedia partitioning of benzene in the Santa Clara Valley is one of the examples provided in the SMCM software manual [4]. We note that due to the lack of adequate information regarding the diurnal variation of emission rate of benzene in the Santa Clara Valley, the average source strength of the sinusoidal source is assumed to be the same as the estimated average emission rate of benzene in the Santa Clara Valley (1206.1 mol/hr) [4]. Moreover, since automobile traffic is an important source for the emission of benzene into the urban atmosphere, the maximum source strength is considered to occur during the traffic rush hours. Accordingly, a 12 hour period per each sinusoidal cycle is used in this simulation with an estimated amplitude of 800.0 mol/hr.

With the above consideration, the calculated dynamic distribution of benzene in the Santa Clara Valley given a 1 ppb initial concentration of benzene in the air phase is shown in Figures 7 and 8. Figure 7 shows the benzene concentration versus time in 6 compartments. Figure 8 is an enlarged display of the benzene concentrations in the air, water and sediment compartments. Since these two figures are in black and white as they appear in this paper, it is difficult to distinguish between

the curves for each compartment. However, when displayed on a color monitor, the curves are easily identifiable. A selected sample of the printed numerical results for the benzene simulation at simulation time of 1000 hours is given in Table 2. From Table 2, we see that the mass of benzene in the air compartment is orders of magnitude greater than that in any other compartment due to the much larger size of the air compartment. It is also noted (Figure 8) that the repetitious sinusoidal source of benzene leads to a clear diurnal variation of the benzene concentration in the air compartment, whereas no clear diurnal variation of benzene concentration appears in other compartments. This stems from the fact that the 12 hour cycle period is not long enough for other compartments to respond to the diurnal cycle observed in the air phase concentration of benzene. Another fact to note in Figures 7 and 8 is that with the exception of the sediment compartment, the remaining compartments appear to approach an apparent steady state. The sediment is slower to respond as a result of the slow diffusion that dominates chemical transport within this compartment.

Finally, we note that the limited field data from the IEMP (EPA's Integrated

TABLE 2

CONCENTRATION AND MASS FRACTION OF BENZENE IN EACH COMPARTMENT AT SIMULATION TIME 1000 HOURS

Compartment	Concentration (gmol/cub-m)	Concentration in Other Units	% Chemical in Compartment
Air	0.471E-07	0.115E+01 (ppb)	0.988E+02
Water	0.136E-06	0.106E+02 (ng/L)	0.187E-01
Soil	0.219E-06@	0.114E+02@ (ng/kg)	0.122E+01
Sediment	0.746E-07@	0.389E+01@ (ng/kg)	0.893E-04
Biota	0.627E-06	0.490E+02 (ng/kg)	0.433E-07
Suspended Solid	0.337E-06	0.176E+02 (ng/kg)	0.232E-06

Total gmols present in the multimedia system = 0.125E+06

@ Average concentrations for the top 10 cm.

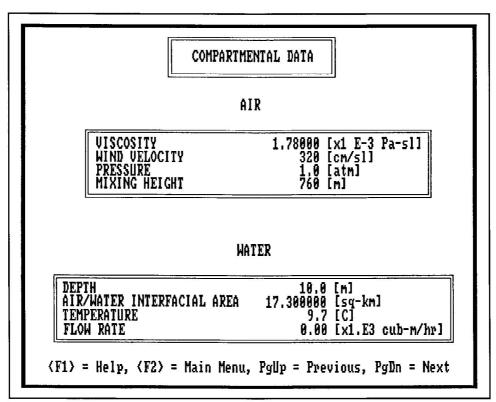


Figure 4 - Data input screen for air and water compartments

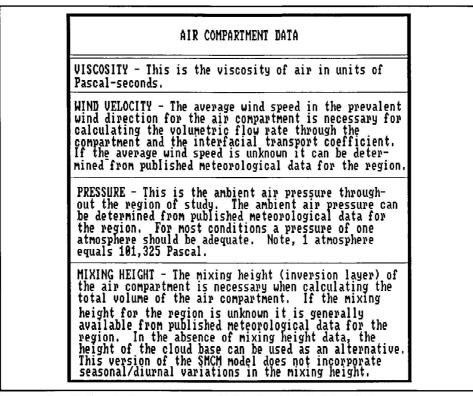


Figure 5 - Online help screen available for the fields of air compartment data in Figure 4

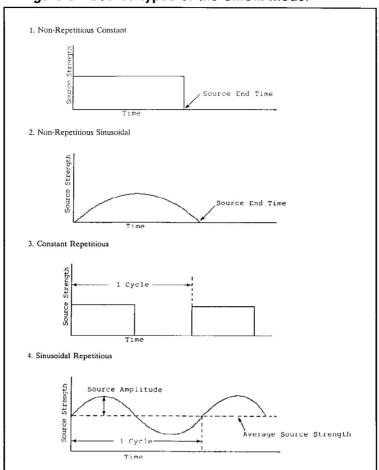


Figure 6 - Source types of the SMCM model

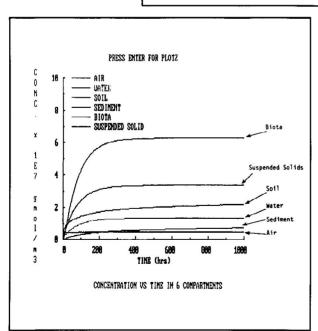


Figure 7 - Distribution of benzene in the Santa Clara Valley: Plot 1

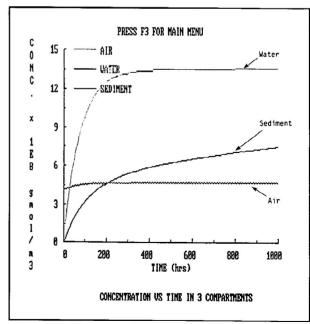


Figure 8 - Distribution of benzene in the Santa Clara Valley: Plot 2

Environmental Monitoring program) [5] study in Santa Clara indicates the air phase benzene concentration to be about 7.7 µg/m3 relative to the calculated value of 3.7 µg/m3. Other limited multimedia measurements of concentrations of trichloroethylene (TCE) and perchloroethylene (PERC) in the Los Angeles and San Diego regions, and TCE in the Santa Clara Valley (California) have been used for model testing [6,7]. These studies illustrated that the SMCM predictions agreed with the available field data within a factor of two to four [6,7], which is better than the accuracy recommended by EPA for screening level models. Therefore, the user friendly SMCM software, with its fast execution and its acceptable accuracy for screening level analyses, makes for an extremely valuable teaching tool.

For More Information on the SMCM Software

The SMCM software (Version 3.0) is available on 360K (2 disk set) or 1.2 Mb 5 1/4 inch floppy disk, or a 720K or 1.44 Mb 3 1/2 inch floppy disk, and includes a user's manual. For more information regarding the SMCM software, you may call the NCITR Office at 213-825-9741 or FAX your inquiry through the same phone number.

Acknowledgement

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Page 26 Spring 1990

The Application of Workstation Technogy in Chemical Engineering

Geoffrey Hulse The Ohio State University

The use of multi-tasking, single-user workstations featuring high resolution, bitmapped displays and some form of windowing system is a well established trend in computing. Although some of the applications developed for this environment are of little benefit to chemical engineers (such as drafting packages), the workstation model in itself represents a valuable new tool to researchers, educators and students alike. At the Koffolt Computer Graphics Lab (KCGL), a facility of the Ohio State University that serves (for both research and educational purposes) the departments of Chemical and Materials Science engineering, we have begun to implement the use of workstations in a manner that encourages users to treat them as a new environment rather than just an oversized terminal.

How does the workstation paradigm differ from the traditional host/terminal configuration and how does it affect the way we do things? In the first place, a user logged in via a terminal may view only one "page" of information at a time, whether it be a graph, source program or error listing. In order to examine something else, he must first erase the current display. This model fails to accommodate the need for humans to operate on a multi-tasking basis; we like to work with many individual pieces in a concurrent manner.

On a workstation, however, a user can view many things simultaneously. Since by definition a workstation must be running a multi-tasking operating system, each window is "live" and continues to execute regardless of the mouse pointer position. This fact may be further enhanced if the operating system imposes a standard architecture to support each application (such as the Digital Equipment Corporation's Compound Document Architecture). One then reaps not only the ability of being able to cut and paste but the additional benefit of one window updating another. At KCGL, for example, a user may copy a graph to the paste buffer, import in into

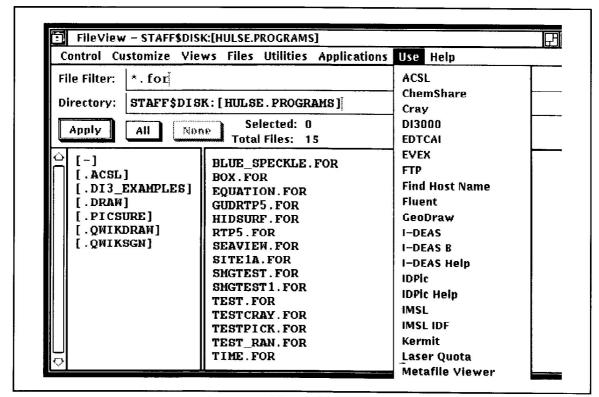


Figure 1

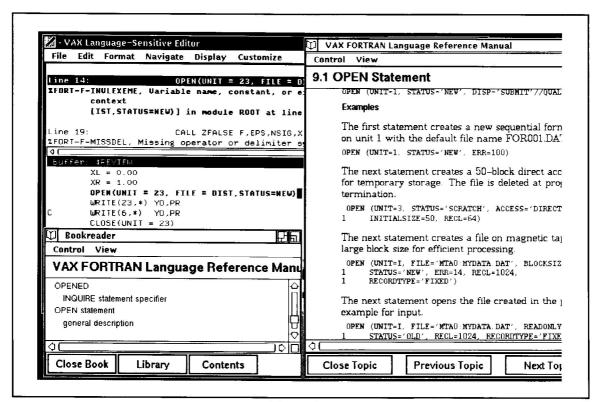


Figure 2

PAINT, through his program one line at a time while to halt execution at a specific line or value and examine variables at that point. All these commands may be performed by clicking with themake notations, then mail the annotated graph to a faculty member who can view the modified image within DEC windows mail. He may also make use of the LiveLink utility within such applications as DEC decision to view instantaneous changes to a chart generated by a spreadsheet as the value of a cell is altered.

In addition to multi-tasking capabilities, workstations frequently offer an improved user interface like DECwindows. A product of the Digital Equipment Corporation, DECwindows is a higher level implementation of the X Window system developed at MIT. Similar interfaces are available from Sun, HP, and IBM, amongst others but I will limit my discussion here to DEC's product since that is what we use at KCGL. The foremost unit within DECwindows is Fileview, a "browser" utility that not only allows a user to perform all tasks from either menus or buttons but displays directory structures in a hierarchical form. The Fileview window is split into two parts with directories on one side and the files of the current subdirectory on the other. By pointing and clicking on a directory name (with a mouse) you move into that subdirectory and its files are displayed accordingly. (see figure 1) You may also select a file by clicking on it, then choose from a pop- up menu of commands appropriate to that file type. (For example, the pop-up menu for an executable image would list RUN but not PRINT as a viable command). In this manner an unsophisticated user can take full advantage of a powerful command lexicon without having to learn exactly what to type for all possible scenarios. On a "dumb terminal", a new user can't even begin to ask for assistance unless he first knows to type HELP. In a DECwindows session, however, the HELP button is always clearly visible at the top of the window.

By exploiting these multi-tasking and system navigation capabilities, the advantages of the workstation environment become apparent. Let us suppose a student has a compilation error in his program. Using the traditional "dumb terminal" model the natural thing would be to print out a listing file, get a copy of the manual (if it is available) and try to find the problem. At KCGL, the same student using a VAXstation running DECwindows could edit his file using the Language Sensitive Editor, compile and review the errors within the same editing session and then use the BOOKREADER application to access a CD-ROM containing the complete FORTRAN manuals, including illustrations. (see figure 2)

Page 28 Spring 1990

Furthermore, the DECwindows interface to the VAX Symbolic Debugger enables a user to step mouse on buttons and/or selecting from menus. The editor may even be left open in another window, allowing the user to concurrently apply fixes to errors detected in the debugging session.(see figure 3) This facility eliminates the need to embed extraneous write statements into a program merely to view suspicious values, a method that was well suited to the era of card readers and batch queues but would appear to be superfluous today.

In chemical engineering we are seeing increased use of methods more commonly thought to be associated with other engineering disciplines. This includes the use of finite element, finite difference programs, pre/post processors and expert systems. Each of these methods has been significantly enhanced as educational tools by the application of workstation technology.

The use of expert systems in chemical engineering has grown dramatically in the past decade. At KCGL, it is now being offered as a technical elective at the undergraduate level. Amongst other things, each student must complete a project written in OPS-5. The current version of this language supports the DECwindows interface (see figure 4), enabling the user to view each of the available tasks as individual windows (session, listener, module,

trace, construct, editor and program i/o). In this manner, a student may make changes to his program whilst viewing the errors and in many cases achieve instant results.

Likewise, the DECwindows interface to I-DEAS Supertab, our pre/post processor for finite difference, finite element modeling has made these packages far more useful as an undergraduate tool. Readily available menus, buttons and other mouse-driven tasks shorten the extensive learning curve that often hampers the value of these programs to undergraduate educators. Furthermore, since each student has a dedicated processor available to his task, jobs run faster. This last point has also improved the usefulness of FLUENT, a fluid modeling package, as it allows students to run more realistic cases and not load down our VAX 8550, where resources must be shared amongst many users.

Even those applications that have yet to produce a window-oriented interface stand to benefit from workstation technology. By merely enabling a user to view output and source code simultaneously, we have enhanced the users ability to debug programs. What's more, the use of onscreen applications like the CALCULATOR, with its ability to cut and paste makes estimating initial values and checking results far easier. One example of this involves theuse of FLOWTRAN, a process

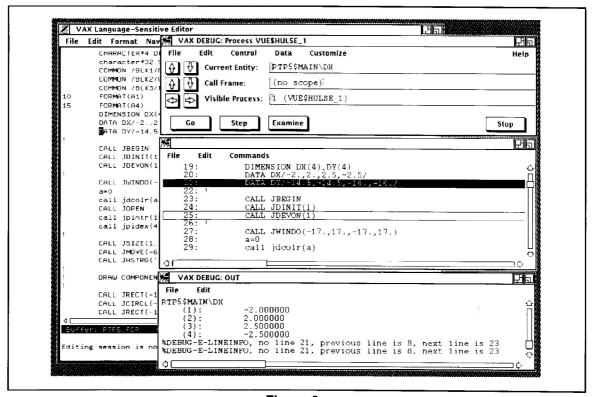


Figure 3

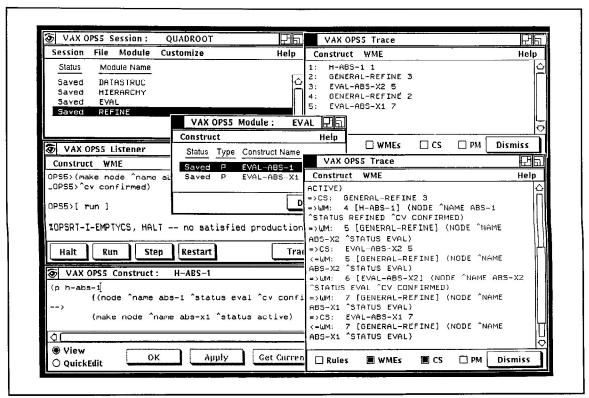


Figure 4

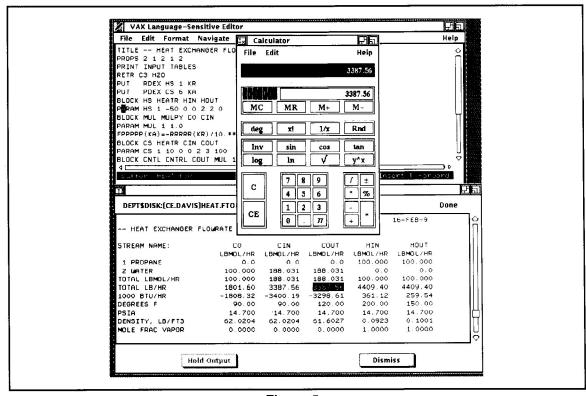
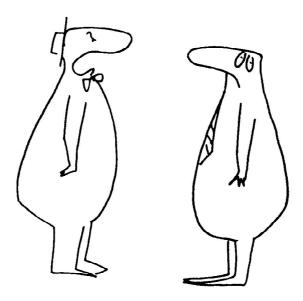


Figure 5

simulator used extensively by the undergraduate design class. (see figure 5).

Conclusion

Numerous applications are being developed for or migrated to the workstation environment. While there are obvious differences between the needs of Chemical engineering and more traditional CADCAM-oriented fields like Mechanical engineering, it is apparent that both stand to benefit from the implementation of a technology that actually facilitates the user's ability to employ it in a constructive manner. Since the undergraduate experience very often establishes habits the student will carry for the rest of his career, exposure to the workstation model in their formative years will enable future engineers to develop work habits appropriate to this new technology.



I can't accept your article on word processors. You wrote it by hand.

CACHE Survey of PC-Based Flowsheet Software

By T. F. Edgar, The University of Texas at Austin

The CACHE Process Engineering Task Force has recently completed a survey of PC-based flowsheeting software. The six packages compared include PC versions of ASPEN (two versions), HYSIM, CHEMCAD, PROCESS, and DESIGN 2000. Mainframe software was not considered in this study. It is clear that with the increasing computational power of PC's, they are becoming a preferred alternative to mainframes because of the attractive feature of interactive input/output using computer graphics or spreadsheets. For PC packages the enhanced user interface, including icons, windows, use of a mouse, and dynamic input with context sensitive HELP, plays a major role in facilitating computer-aided design.

CACHE has also received information on new educational discounts on several of the packages, some of which are significant reductions from previous prices. A summary of the software packages, their key features, and prices is given on the following pages. Chemical engineering faculty are encouraged to contact individual company representatives about more details; their addresses and phone numbers are provided below.

Company Contacts:

Joe Sontheimer ChemShare P.O. Box 1885 Houston, TX 77251 (713) 627-8945

Randall P. Field Aspen Technology, Inc. 251 Vassar Street Cambridge, MA 02139 (617) 497-9010

George Kasse SIMSCI 2950 North Loop West Suite 830 Houston, TX 77092 (800) 231-2754 Nathan Massey Coade/Chemstations 10375 Richmond Avenue Suite 1225 Houston, TX 77042 (713) 973-9060

Michael Mendelson JSD Simulation Service Company 6000 East Evans Ave., Building 3 Denver, CO 80222 (303) 758-6862

Dr. Bill Svrcek Hyprotech 119 14th Street NW #400 Calgary, Alberta T2N1Z6 CANADA (800) 661-8696

Page 32 Spring 1990

PC-Based Flowsheet Simulation Software Packages

Version	CHEMCAD (2.3)	SIMSCI* (2.01)	CHEMSHARE
Required RAM	640K	640K or	(5.0) 2Mb
		4 Mb	
Required disk storage	3Mb	12.5Mb or 20Mb	15Mb
Required processor	8088, 80286 or 80386	80286 or 80386	80386
Required coprocessor	8087, 80287, or 80387	80387	80387
Operating System	DOS	DOS or UNIX	DOS
Recycle convergence enhancements	Y	Y	Y
graphical input	Y	Y	N
interactive input	Y	Y	Y
help screens	Y	Y	Y
process flow diagram generations	Y	Y	Y
number of components (phys. prop. library)	600	1200	1000
security	kcydisk	hardware device	hardware device
group contribution K values	Y	Y	Y
Unit operations			
rigorous fractionation	Y	Y	Y
pumps, compressors, mixers	Y	Y	Y
heat exchanger	Y	Y	Y
reactors	Y	Y	Y
Educational user cost	\$1,200/yr (unlimited number of keydisks)	\$600 (1st 2 copies) \$100 (each additional copy)	\$5,000
Y = yes, $N = no$	*2 versions, PROCESS and PRO2		(continued on next page)

CACHE News

PC-Based Flowsheet Simulation Software Packages (cont'd)

Version	HYSIM "C" (C1.15)	Aspen Plus (Model Manager)	Aspen/SP-38 (7.0)
Required RAM	640K or 3 Mb (386Version)	4-5Mb	4Mb
Required disk storage	4Mb	20-40Mb	25Mb
Required processor	8088, 80286, or 80386	80386	80386
Required coprocessor	8087, 80287, or 80386	80387	80387
Operating System	DOS	DOS	DOS
Recycle convergence enhancements	Y	Y	Y
graphical input	Y	Y	Y
interactive input	Y	Y	Y
help screens	Y	Y	N
process flow diagram generations	Y	Y	Y
number of components	850	1500	>1500
security	hardware device	hardware device	hardware device
group contribution K values	Y	Y	Y
Unit operations			
rigorous fractionation	Y	Y	Y
pumps, compressors, mixers	Y	Y	Y
heat exchanger	Y	Y	Y
reactors	Y	Y	Y
Educational user cost	\$500-1st copy, \$200 each copy 2-4, \$100 each additional copy	\$1,000 for first copy; additional student copies available at \$100 each	\$4,000

Page 34 Spring 1990

Y = yes, N = no

Microcomputer Chemical Engineering Programs (developed by Professors)

Edited by Bruce A. Finlayson

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 will not be accepted. This requirement has two goals: to reduce the need for additional typing and to encourage academic chemical engineers to use electronic mail. Since anyone writing a computer code is computer literate, they can figure out how to use BITNET at their local installation when the incentive is exposure of their program. They can then share the protocols with their colleagues for other uses.

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



The Kinetics and Selectivity of Consecutive Reactions

By Alvin H. Weiss and Reynold Dodson

This program was designed for use by Chemical Engineering students of kinetics and Reactor Design in both the undergraduate and graduate courses at Worcester Polytechnic Institute. Three reaction systems are provided:

$$k_1$$
 k_1 k_1 k_1
 $A ext{-->} B$ $A + H_2 ext{-->} B$
 k_2 k_2 k_2
 $B ext{-->} C$ $B + H_2 ext{-->} C$
 k_3
 $C + A ext{-->} D$
 k_4
 $B + B ext{-->} D$

The absolute values of k₁ and the relative values of k₂, k₃, and k₄ to k₁ can be set for any starting mixture. Plots of concentration vs. time are generated and the time necessary to obtain maximum yield of intermediate is found. Reaction paths of composition vs. conversion are plotted, and the maximum selectivity and conversion are indicated. The student or practicing engineer can use the plots to establish relative rate constants and kinetics corresponding to experimental data; and from these predict when and at what conversion maximum yield is had as a function of reaction feed composition.

The program is written in PASCAL, supports a math coprocessor, and utilizes an Intel 80286 coprocessor. MS-DOS, 512 KB RAM, and one-disk drive are needed. Display is either color or black and white. A disk and descriptive information may be obtained for \$12.00 by writing to:

Professor Alvin Weiss, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609. Specify 3-1/2" or 5-1/4" floppy.

Equations of State

By Kenneth R. Jolls

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 temperature. Overall property ranges are user options.

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 64OK RAM and EGA-level graphics. A math coprocessor is recommended.

Descriptive information may be requested 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. You can also obtain information about them from the conference "Chemical Engineering Software" on the Bulletin board GRAND@LSUCHE. To get started, send a Bitnet message:

To: Grand@LSUCHE From: person id@node id help

- 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, Alan Foss, University of California, Berkeley
- 13. Real-time Dynamic Distillation Simulation and Relative Gain Program, No. 27 and 28, Alan Foss, University of California, Berkeley

Page 36 Spring 1990

ANNOUNCEMENTS

Electronic Mail Task Force

The Electronic Communications Task Force (Joe Wright, Norm Rawson, John Hale, John Hassler, Robert Brodkey, Wayne Crowl, and Peter Rony) of CACHE is in the process of performing major revision and updating of its on-line electronicmail nickname (alias) and FAX listings for IBM mainframes and VAX minicomputers. Our task force objectives are (a) to collect email userid and FAX information that would be incorporated in the 1990-1991 Chemical Engineering Faculties (Volume 39); we wish to produce the most comprehensive listing of academic electronic mail userids available to date: (b) to verify the accuracy of each departmental userid listing; (c) to identify one individual (for example, the department head, a faculty member, or a secretary) in each department who would be charged with the responsibility of receiving professionally-appropriate, globally-broadcast messages (for example, from AIChE headquarters or the programming committees of AIChE divisions) and respond to them quickly; and (d) to place each list in a form such that it can be more easily accessed by search routines. Once created, the updated listings will be available as electronic files--RONY NAMES A0 for the IBM and BRODKEY NAMES A0 for the VAX-that can be obtained by sending a request to RONY at VTVM1.

This email message or letter is being sent to one faculty member--preferably an individual who uses electronic mail regularly--in each domestic and international chemical engineering department. We request that you identify somebody in the department who would provide us with a complete listing of verified departmental faculty electronic mail userids and FAX numbers for 1990-1991. Please send the list to me either by email or by post. If you would like to automatically receive the electronic update, please let me know. Thank you for your assistance.

Peter R. Rony
Department of Chemical Engineering
Virginia Tech
Blacksburg, Virginia 24060
BITNET: RONY at VTVM1
FAX: no departmental FAX avail.
Phone (work): (703) 231-7658

Phone (home): (703) 951-2805

SpeedWACS

SpeedWACS is an interface between the chemical process simulation package SpeedUp and IBM's Advanced Control System (ACS). It provides the customer with the ability to run SpeedUp simulations under the control of ACS. These simulations have access to all of the process information contained in ACS's database and in turn the simulation can be controlled by any of ACS's control facilities. From ACS's perspective the simulation appears to be a real plant putting measured data to the database. From SpeedUp's perspective the data receiveed from ACS is SET (constant) data used for the duration of the steady state run or used for the duration of the time step for a dynamic simulation. You can create any of the simulation types allowed by SpeedUp including Steady state, Optimization, Parameter Estimatin and Dynamic simulations. applications are nuimerous including online data reconciliation, online parameter estimation, online optimization, model based control, constrained control, operator assisted control and operator training.

SpeedWACS utilizes SpeedUp's External Data Interface facilities. To define a SpeedWACS simulation you simply add an EXTERNAL section to an existing SpeedUp simulation prefixing all tags with the characters ACSxxxxx where xxxxx is the SPL number of the desired SPL program. RECEIVEd variables are obtained from ACS and TRANSMITed variables are put to the ACS database. Once the EXTERNAL section has been defined you set the EXTERNAL option in the OPTIONS section and RUN the problem. SpeedUp recognizes the ACS prefix and takes appropriate action to create a SpeedWACS module and copy the required datasets. You then define the SPL program to ACS through the PG form and execute the simulation from the XX3 display or via any method normally used to run an SPL program.

For questions and support contact:

Dennis Herman
Waterloo Centre for Process
Development
University of Waterloo
200 University Ave W.
Waterloo Ontario N2L 3G1
ph (519) 885-1211 x3300 or x2947
fax (519) 888-6179

ANNOUNCEMENTS (continued)

Chemical Engineering Progress has published their 1st Annual Software Directory. Address requests to Chemical Engineering Progress, 345 E. 47th St., New York, NY 10017.

Instruction Delivery Systems is a new magazine devoted to the issues and applications of technology to enhance productivity in education, training, and job performance. It is published bimonthly by Communicative Technology Corporation, 50 Culpeper Street, Warrenton, VA 22186. Subscriptions are free to qualified professionals, \$15 per year for others plus \$5 for other countries.

FOURTH WORLD CONGRESS OF CHEMICAL ENGINEERING

16-21 June, 1990 Karlsruhe, Federal Republic of Germany

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Please submit title and abstract (1 page) by mail or by fax to:

Richard S. Mah
Department of Chemical Engineering
Robert R. McCormick School of
Engineering and Applied Science
Northwestern University
Evanston, IL 60208-3120

TELEPHONE: (708) 491-5357

FAX: (708) 491-3728

before June 15, 1990, on any of the following topics: Information networks, databanks, expert systems, process analysis, synthesis, control, simulation and optimization.

Page 38 Spring 1990

LET US HEAR FROM YOU

What would you like to see made available in the way of CACHE products and services? CACHE is interested in your needs and opinions! Tell us a bit about your courses and what educational and computer oriented materials would assist you in doing a better job, make the courses more interesting, and/or save you time and money.

Are you interested in obtaining

- course supplements in the form of software?
- educational modules?
- booklets?
- homework assignments?
- or?

Detach and mail to:

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

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

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Spain

University of Maribor, Yugoslavia

Topics in this issue of the CACHE Newsletter:

CACHE Curriculum Task Force

A User's Guide to Electronic Mail (Part 2)

Partitioning of Pollutants in the Multimedia Environment: The SMCM Software

The Application Of Workstation Technology In Chemical Engineering

CACHE Survey of PC-Based Flowsheet Software

Microcomputer Chemical Engineering Programs

Announcements

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