CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 29

Fall 1989

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PRESIDENT'S PERSPECTIVE

H. Scott Fogler
University of Michigan

H. Scott Fogler is currently President of CACHE Corporation and Professor and Chair of Chemical Engineering at The University of Michigan. He is author of two textbooks and over 90 research publications in the areas of flow and reaction in porous media and colloid stability.

We will soon be approaching the 25th Anniversary of the CACHE Corporation. As we look back over the years we see many major accomplishments, such as disseminating FLOWTRAN and developing the associated educational materials, the CHEMI Modules, the case studies, the monographs on real time computing and on AI, the interactive computer modules, and many others. Rather than dwell on our past achievements, however, the organization is looking to the future to envision where CACHE will be in 1999 with respect to its mission, focus, and service to the profession. To answer these questions, the primary agenda item of the last meeting of the CACHE board of trustees was a focus on the future directions of CACHE over the next 5, 10, and 15 years. In order to achieve this, Eastman Kodak was kind enough to provide a facilitator who is an expert in leading discussions on "*futuring*." Futuring exercises provide a framework to describe the characteristics of what we envision 10 years or so from now.

While there are many models used for "futuring," the one we used was an organizational assessment model focusing on Suppliers, Inputs, Processes, Outputs, and Customers—SIPOC Model. Prior to the meeting, many chemical engineering departments were surveyed to determine how CACHE could be most useful to them. While there is not sufficient space in this column to describe all of the exciting possibilities discussed at our meeting, a few of the things we see in the near future include electronic journals, textdisks (as opposed to textbooks), interactive video-disks, wide use of the electronic chemical engineering bulletin board to obtain home problems and recent research results, video windows, easy access to a large number of data bases, satellite CACHE conferences, modular based software and videoware, and perhaps a more focused CACHE portfolio.

I now would like you to turn your attention to three new projects in which CACHE is a participant with chemical engineering departments at three different universities that focus on the more immediate future. All of these projects were recently funded by the National Science Foundation.

Purdue University-NSF-CACHE Initiative "Industry ChE Laboratory Module Development"

Chemical Engineering laboratory experience is required in all accredited chemical engineering curricula. Such laboratories, along with senior design courses, are often the "capstone" courses which not only draw on previous chemical engineering course material, but also require the students to use statistical analysis, written and oral communication skills, and since the lab is usually a group effort, interpersonal skills.
This project is a novel approach to the design of experiments for the senior ChE laboratory which - by combining computer simulation, the cooperation of industrial co-sponsors, and a videotaped facilities tour - will result in a laboratory experience which is more challenging, interesting and educationally effective.

The ideal laboratory experiment would duplicate a real industrial project. The students would use modern equipment to investigate a complex and challenging problem, and would do so under realistic time and budget constraints. We are working with industrial sponsors to develop computer simulation modules of real industrial processes to be used as laboratory experiments in the senior ChE laboratory. Each sponsor will also furnish a 20-minute video tape showing plant equipment, control displays, and flow diagrams, indicating operating flows, temperatures, pressures, etc. In addition, the company will furnish typical costs and time requirements of experiments which the student will use in solving the problem. With these modules, the emphasis is shifted from the traditional experimental problems associated with running real equipment, to problems of planning proper experiments and data analysis. Since each exercise is *open-ended*, and a variety of experimental options are available to the

student with associated costs and time requirements, the student must carefully choose his/her set of experiments to meet the overall budget and time deadlines.

To date, five companies (Amoco, Dow, Mobil, Tennessee Eastman, and Air Products) have sponsored modules. These five modules are all in the more traditional ChE areas of reactor design, separations, and heat transfer, however at least two more modules will be added in non-traditional areas.

University of Michigan-NSF-CACHE Initiative "A Focus on Developing Innovative Engineers."

As we find ourselves in a time that has been described as the era of the "knowledge explosion", much akin to the "industrial revolution," we need to re-examine our teaching roles as we focus more on developing the students' "life-long learning and creative skills." In the future we must place greater emphasis on developing the students' divergent thinking skills. The goals of this project are not only to develop educational materials designed to enhance innovation in the core chemical engineering courses but also to devise an interdisciplinary model for increasing students' innovative skills. To achieve these goals, we are developing open-ended problems and interactive computer modules together with problem-solving heuristics. The open-ended problems are based on real technological issues encountered in companies such as duPont, Eli Lilly, Amoco, Dow Corning, and Upjohn. We are designing these problems to be course-specific: the use of lasers to melt and cut videotape is explored in the transport phenomena course; methods of removing entrained catalysts in catalytic cracking operations are generated in the fluid mechanics course; and novel methods of adding vitamins to cereals are devised in the first chemical engineering course. With these educational aids, students can practice design creativity in each chemical engineering course rather than just in a single capstone course. Such practice in using higher level thinking skills is analogous to the traditional practice of reinforcing lower level thinking skills gained through close-ended home and exam problems which reinforce the concepts discussed in class.

In addition to the open-ended problems, we are developing 3 to 5 interactive computer simulations for each chemical engineering course. The students' decision making and divergent thinking skills are exercised and enhanced by providing a large number of branch points in these simulations. Each menu-driven simulation reviews the pertinent fundamentals, interactively tests those fundamentals, and provides a demonstration, followed by an interactive exercise with branching components together with the problem solution and an evaluation of the student's performance. To date, 5 interactive computer modules have been developed for the first chemical engineering course (Stoichiometry - Material and Energy Balances) along with 2 for the fluid mechanics course.

University of Washington-NSF-CACHE Initiative "Graphical Computer Aids for Chemical Engineering Education"

This project will produce a set of computer programs that permit easy use, and quick, easy interpretation of the results aided by post processing and graphical output. The program applications are divided into two general areas: (1) reactor design and (2) fluid mechanics, heat and mass transfer, and their combination. The reactor design programs will permit the calculation of conversion and temperature for realistic reaction systems when any or all of the following phenomena are important: axial dispersion, radial dispersion, and heat/mass transfer resistances for catalyst pellets. The output of these programs can be presented graphically, so that three-dimensional perspective views and two-dimensional contour plots can be made on demand. The software will also allow the calculation and graphical display of the sensitivity of the results to the parameters of the problem, and the detailed investigation of each term in the equation (to help if when the corresponding phenomenon is important). The fluid flow programs will permit the easy, graphical input of a finite element mesh, the solution of any combination of the Navier-Stokes equations, the energy equation, and the diffusion-concentration equation, along with chemical reaction. The post-processing graphical display will show streamlines, stress lines, vorticity, viscous dissipation, etc. in the same 3D perspective or 2D contour diagrams. Students will also be able to generate plots of each term in the equation so that they can see via graphs the important terms. The expected benefits to a student include an improved understanding of basic chemical engineering phenomena by the student, an increased ability to think while developing and testing computer models, more realistic design of chemical reactors, enhanced productivity skills in design, and the inclusion of design problem situations involving transport limited situations.

Each of the above NSF projects were funded between two to three years. Each project has a steering committee consisting of faculty from different universities. It is expected that class testing of the materials for some of the projects will begin during the coming year. Anyone interested in participating in the test or obtaining more information on any of these projects, please contact either myself or David Himmelblau, executive

officer of CACHE.

Futuring

Finally, let me return to the concept of "futuring." Recently I had the opportunity to go through the "futuring" exercise used by Dow Corning to suggest courses of action and directions. This exercise used Joel Barker's book and videotape "Discovering the Future." I would like to share a few of the ideas as we examine the directions of both our profession and our roles as professors. Specifically, Barker speaks of the concepts of **paradigm shifts**, **paradigm paralysis**, and **paradigm pioneers**. A paradigm is a model or pattern that is a set of rules that defines boundaries and tells what to do to be successful at these boundaries. Success is measured by the problems you solve using these rules and regulations. When a paradigm shifts, everything goes back to zero; it does not matter what your past successes were, everyone is on equal footing. Barker uses the example of the Swiss watch industry to make this point. In 1968 the Swiss had approximately 80% of the world market in watch sales and were known for their fine history of quality watches. Today they have below 10% of the market because of the emergence of quartz digital watch, yet...they were the ones who invented the quartz digital watch!! However, they were caught in a "paradigm paralysis" and thought that what was successful in the past would be successful in the future. After all . . . the digital watch didn't have a main spring; it didn't tick; ***who*** would buy such a watch? Consequently, they left their invention unprotected without a patent, and you know the rest of the story. Seiko of Japan and Texas Instruments picked up the idea and capitalized on it. The employment in the Swiss Watch industry dropped from about 65,000 to about 15,000 in a period of little over 3 years. The paradigm shifted and the success of the Swiss in the past were irrelevant; everything went back to zero!

In regards to engineering education, we have all heard many of our colleagues say, "Our students are turning out OK. Why should we change what we are doing now?" Are we perhaps caught in a "paradigm paralysis?" To break out of a paradigm paralysis requires what Barker calls "**Paradigm Pioneers.**" Paradigm pioneers have the courage to move forward even though all the evidence isn't in that they will succeed in their endeavor.

A Paradigm Shift?

Many feel that our profession is in transition and that we are waiting for the next paradigm shift. We see competition from our sister disciplines in areas that we believe might well be chemical engineering based. A few examples include optical fibers and chemical vapor deposition in Electrical Engineering, ceramic processing by the Materials Engineering Departments, and environmental engineering by Civil Engineering. In fact, some of our colleagues have suggested writing a book entitled, *"The Ones That Got Away from ChE."* describing the research areas that have been picked up by other disciplines.

Over the summer, I have come to the conclusion that a very small but significant paradigm shift has occurred in the teaching of our basic chemical engineering courses. The shift has been brought about by the recent introduction of *fantastically user-friendly* software packages containing ordinary differential equations solvers, least squares analysis, polynomial fitting, and linear and non-linear equation solvers. The same type of paradigm shifts have occurred in the past as we went from **slide rules** to **calculators** to **PC's** and now to **user friendly PC applications.** With each change, the type of problem we are able to assign changes along with the enhanced ability to *explore or play with* the problem. This characteristic is certainly true in chemical reaction engineering, we can now focus on setting up complex problems such as multiple reactions, reactors with pressure drop and heat exchange, and other topics requiring the solution to simultaneous and/or nonlinear ordinary differential equations. I have been using one software package that I believe will increase, by perhaps an order of magnitude, the complexity of the homework problems that we now are able to assign. Such a package allows for easy parameter evaluation so that the student can study trends and parameter sensitivity. Students then can describe the trends they see by the varying parameters in their equations, eg., what is the effect of varying the diameter, and the rate and transport coefficients in a membrane reactor? In addition, least square analysis, polynomial fitting and differentiation of data can easily be used to determine rate laws. Similar applications of these software packages exist in transport phenomena, thermodynamics, fluid mechanics, and separation processes. CACHE is currently negotiating for the distribution of one such software package, POLYMATH, to all CACHE supporting departments, and we hope to have this package available sometime in the near future. I expect it will have a major impact on our teaching and our students.

What other paradigm shifts are occurring in chemical engineering? Everyone is looking for the next paradigm shift in Chemical Engineering Research. Which new research directions will ChE take: Superconducting materials? Safety? Microenvironmental engineering? Perhaps we need to expand our thinking. Could the **next paradigm shift** be the manner in which we teach our students?

CACHE Artificial Intelligence in Process Engineering Task Force

James F. Davis, Ohio State University
George Stephanopoulos, MIT

The AI in Process Engineering Task Force

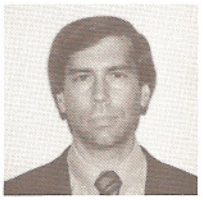
The re-emergence of Artificial Intelligence in the early part of this decade has now significantly challenged the conventional modes of engineering work and education in chemical engineering. Back in Autumn 1985 when the effects of this technology were surfacing and when the first AIChE session on AI was held, CACHE formed an ad hoc committee to study the role of AI in chemical engineering. In anticipation of the apparent and rapidly growing importance of the technology at that time, this committee came together in Spring 1986 to identify how CACHE can play a role in fostering the introduction and dissemination of this new technology for educational purposes.

In just a few years since these initial meetings, chemical engineering has seen the role of AI make the transition from a research topic only into a viable technology in industry and take on a rather pervasive nature as an important problem-solving tool for many types of applications. A considerable amount of early hype has settled into a realistic perspective for a useful technology. Hardware platforms have changed dramatically towards general purpose workstations and software has evolved into packages with sophisticated graphics interfaces, a variety of knowledge representations and inferencing strategies and flexible features allowing ready integration. Courses in artificial intelligence, once the sole domain of computer science and directed toward research are now being made available in chemical engineering curricula as technical electives to graduate and undergraduate students.

In responding to these very rapid changes, the ad hoc task force was recently formalized as a CACHE task force and has increased in size as a result of a growing interest in AI among academic institutions. In the three years since its inception, the AI in Process Engineering Task Force has spearheaded several activities which have broadly promoted the role of AI in chemical engineering education and have recently

Task Force Members

George Stephanopoulos is the J.R. Mares Professor of Chemical Engineering at Massachusetts Institute of Technology (Diploma Chemical Engineering from National Technical University of Athens; M.E. from McMaster University; Ph.D. from University of Florida). Professor Stephanopoulos' principal interests are in the areas of product and process design, and process operations and control, with particular emphasis on the use of computer science and technology in solving problems in the above areas. Through MIT's Leaders for Manufacturing Program, he is involved with studies at the interface of engineering and management. He is the author of the text, *Process Control: An Introduction to Theory and Practice*. He received the Dreyfus Scholar, Colburn and C. McGraw Awards.



Jim Davis is an associate professor of Chemical Engineering at the Ohio State University (B.S. from U. Illinois; M.D., Ph.D.. from Northwestern University). Jim's research work is in application of Artificial Intelligence to process operations and design. At Ohio State, he heads the AI in Chemical Engineering groups within the Laboratory for AI research. He has strong interests in computer applications both in research and teaching and his primary teaching responsibilities include process control, process design and expert systems in process engineering. Jim was elected to the CACHE board of trustees in November 1987 and is presently involved with the Task Force on Artificial Intelligence in Process Engineering.

Prof. Venkat Venkatasubramanian is an Associate Professor in the School of Chemical Engineering at Purdue University. He obtained his Ph. D. in chemical engineering from Cornell University. Venkat worked as a Research Associate in the Department of Computer Science at Carnegie-Mellon University and also taught at Columbia University before joining Purdue. At Purdue, Venkat directs the research efforts of several graduate students and coworkers in the Laboratory for Intelligent Process Systems. This laboratory has several ongoing projects on the application of knowledge-based systems and neural networks to various problems in process diagnosis and control, product design, and process operations. In the area of teaching, Venkat has authored a three-volume CACHE case study on knowledge-based systems for heuristic classification problems in process engineering. Venkat has also taught AI courses at Columbia University, University of Notre Dame, M.I.T., University of Thessaloniki (Greece) and in chemical companies for an audience of academic researchers and industrial practitioners.

produced a number of products which address education tangibly.

The table below lists the participating members of this task force.

The Role of Artificial Intelligence in Chemical Engineering Education

The mission of the task force is to address the role of AI and its derivative environments in the education of chemical engineers. This mission was succintly scoped by Joe Wright of Xerox with the following series of precepts and corresponding questions:

1. Chemical engineers are problem solvers: How can AI help in teaching problem solving?

2. Computers are and will be pervasive in every aspect of engineering: How will AI impact how computers are to be used?

3. Current and future engineering needs are and will be increasingly multi-disciplinary: How does AI aid in the application of general knowledge to new problems?

4. Engineering work is based on increasingly larger amounts of information: How will AI help to handle these large amounts of information?

5. Fundamental science is the source of innovation: How can AI play a role in making it active within the scope of engineering problems?

These questions have served to focus the current efforts of this task force on several specific elements of teaching. Most prominant is the use of AI-based techniques and methodologies in the teaching of problem solving. It is recognized that AI methodologies emphasize the identification of specific types of knowledge, the organization of knowledge and the strategies for using knowledge to solve problems. AI, therefore, provides a precise means of articulating how to do problem solving. In terms of education, the specific motivations for the current activities of the committee have therefore centered around a concensus that AI techniques will impact teaching by offering improved ways for:

1. Formalizing tasks, knowledge, problem formulations and solutions,

2. Conceptualizing problem-solving models and methodologies,

3. Applying problem-solving models to different applications,

4. Enhancing analytical abilities.

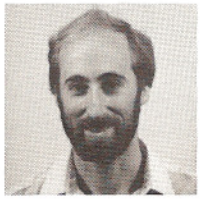
CACHE Products Available

To date, the mission and goals described have led to three categories of products from the AI in Process Engineering Task Force.

1. Special Issue of Computers and Chemical Engineering

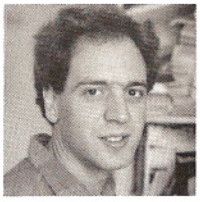
An initial objective of the task force was to generate a compilation of current AI research projects in chemical engineering. The purpose of this compilation was to provide a comprehensive and current view of a developing but as yet immature field. Although much has changed even since the publication of the Sept/Oct 1988 issue, the collection of articles still offers a broad perspective on the challenges facing the application of AI in chemical engineering.

The guest editors, George Stephanopoulos of MIT



Lyle H. Ungar did his undergraduate work at Stanford and doctoral studies at M.I.T., both in chemical engineering. He is currently on the faculty at the University of Pennsylvania. He has received the Presidential Young Investigator Award. Lyle's current work focuses on the use of artificial intelligence and neural networks for fault diagnosis and process control. As part of this work, he and his students are developing a "computerized process engineer" which uses first principles reasoning to analyze chemical plants.

Mark Kramer is Associate Professor of Chemical Engineering and Associate Director of the Laboratory for Intelligent Systems in Process Engineering (LISPE) at the Massachusetts Institute of Technology. Professor Kramer received his Bachelor's degree at the University of Michigan and his PH.D. from Princeton University, both in chemical engineering. His major interests are in the application of new and traditional computer techniques to problems of process operations, including fault tolerant control, intelligent process monitoring, alarm handling, and safety analysis. Professor Kramer has been active in these areas since joining M.I.T. in 1983.



Michael L. Mavrovouniotis is an assistant professor at the Chemical Engineering Department and the Systems Research Center of the University of Maryland, College Park. He obtained his Ph.D. from the Massachusetts Institute of Technology. His general research interests are in Computer-Aided Engineering of Chemical and Biochemical Processes, with emphasis on Symbolic Computing and Neural Networks. His current projects include Identification of Metabolic State of Bioreactors; neural networks for monitoring complex dynamic systems; and prediction of properties of substances from their molecular structure.

and Michael Mavrovouniotis with the University of Maryland, collected 15 papers by a variety of people working in the field. As a collection, the papers were and still are representative of the breadth of current research and development in progress. Covered in the papers are the following subjects:

1. Alternative schemes for modeling the behavior of physical systems,
2. Design of databases for engineering activities,
3. Methodologies for engineering design,
4. Diagnostic strategies,
5. Planning and scheduling of process operations.

To obtain this special issue, the reference is: "*Artificial Intelligence in Chemical Engineering—Research and Development*," Computers and Chemical Engineering, vol.12, 9/10, September/October (1988)

2. Case Studies

To provide chemical engineering faculty and students with detailed accounts on how various AI methodologies can be used to solve chemical engineering problems, a series of three case studies have been published. These case studies were drawn from projects in an expert system course taught by V. Venkatasubramanian who is presently with Purdue University. Each of the case studies includes:

1. Methods for representing the knowledge.
2. Details on the search methodologies used.
3. Lists of rules and their structural organization.
4. Details on the computer implemenation.
5. Alternative scenarios to be explored.

Authored by V. Venkatasubramanian and edited by George Stephanopoulos, the three case studies are as follows:

1. CATDEX: An expert system for troubleshoot ing a fluidized catalytic cracking unit
2. PASS: A Pump selection expert system
3. CAPS: An Expert System for Plastics Selection

The case studies are sold on an individual basis at a unit cost of $20 for CACHE supporting institutions and $35 for non-supporting institutions. Individual volumes are $10 each for CACHE supporting institutions and $17 each for non-supporting institutions. They can be obtained from:

CACHE Corporation
P.O. Box 7939
Austin, Texas 78713-4933
(512) 471-4933

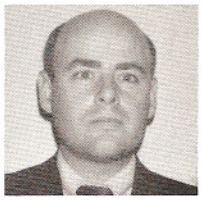
3. A Series of Monographs on AI in Chemical Engineering

Two years ago the task force commissioned a series of monographs on AI in chemical engineering as a mechanism for disseminating detailed information. These monographs have been and are being written for use as main or supplementary material in advanced undergraduate and graduate courses or as an introduction to AI by practicing engineers. Three monographs in the series will become available this fall. The purpose of the first three monographs is to provide detailed discussions on the principles, ideas, techniques and methodologies of AI as they apply to chemical engineering. Later monographs will address approaches to specific problems of direct interest to chemical engineers such as fault diagnosis, design, etc.

Volume I, entitled, "*Knowledge-Based Systems in Process Engineering: An Overview*," is authored by George Stephanopoulos of MIT. This volume serves as

Ali Cinar is currently an associate professor at Illinois Institute of Technology. His research interests are chemical process control and artificial intelligence applications. His teaching activities include process design, process control, expert systems courses and development of computer interfaced experiments in reaction engineering and process control. Dr. Cinar received his B.S. in chemical engineering from Robert College, Turkey. After completing his Ph.D. studies at Texas A&M University in 1976, he became a faculty member at Bogazici University, Turkey. He spent a year as a visiting faculty member at the University of Wisconsin, Madison in 1981, before joining the Illinois Institute of Technology in 1982.

Aydin K. Sunol received his undergraduate education in Chemical Engineering at Bosphorus University, Istanbul, Turkey. He has graduate degrees in Industrial Engineering and Chemical Engineering from England and the USA. After obtaining his chemical engineering doctorate in 1982 at VPI&SU, he joined the chemical engineering faculty at University of South Florida where Aydin is an Associate Professor since 1986. Currently, he is on leave at Systems group at ETH Zurich, Switzerland. Aydin teaches undergraduate and graduate courses in process design and separation processes. His reaearch interests are in processing systems engineering and supercritical extraction. He is a member of AAAI, AIChE, ACS, NPSE, and Sigma X.



Bradley R. Holt is an assistant professor of Chemical Engineering at the University of Washington. He received his B.S. in chemical engineering from the University of Minnesota in 1979 and his Ph.D. from the University of Wisconsin in 1984 when he joined that faculty at Washington. His research interests include linear, nonlinear and batch aspects of process control as well as the development of neural networks for system identification and the interpretation of spectra.

an introduction to the monograph series and provides a broad perspective on AI. Specifically, this volume addresses the scope, history and market of AI and defines the need and role of knowledge-based systems in chemical engineering. Particular attention is paid to describing the general issues surrounding software and hardware environments.

Volume II, entitled, "*Rule-Based Expert Systems in Chemical Engineering*," is authored by James F. Davis and Murthy S. Gandikota of Ohio State University. This monograph focuses specifically on the implementation of knowledge-based systems in rule-based languages. The emphasis is not on the mechanics of rule-based programming environments, but on the issues which impact the implementation and performance of a system. Using specific examples, the monograph covers these issues in detail. As a stand alone chapter, several of the most popular methods for various kinds of uncertainty handling are discussed and compared.

Volume III, entitled, "*Knowledge Representation*," is authored by Lyle Ungar of the University of Pennsylvania and V. Venkatasubramanian of Purdue University. The content of this monograph is directed at two distinct aspects of knowledge representation. In the first part of the monograph, the problem-independent issues and features of a variety of knowledge representations are presented. Included are discussions on semantic networks, frames, scripts and object-oriented programming. The second part addresses the subject of qualitative physics applied in chemical engineering. The issues of representing structure and behavior are discussed in detail. Examples demonstrating two philosophies are used to illustrate advantages and limitations.

The monographs will become available this fall from CACHE at the same address listed for the case studies. The unit cost is yet to be determined.

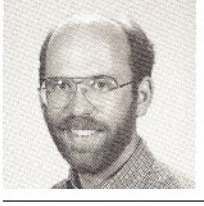
Future Directions for the Task Force

As with technology, the AI in Process Engineering Task Force is a relatively young task force in CACHE. While there have been a number of accomplishments, the task force is still in the process of deciding upon and undertaking new initiatives which are aimed at the goals outlined above. Current plans include the continued development of the monograph series with an emphasis on specific chemical engineering problem areas and the continued development of additional case studies. New initiaitives on the agenda include the establishment of a users group of educators with interests in AI applications and the dissemination of short examples on the use of AI, designed to complement the teaching of traditional chemical engineering science courses.

For further information on this task force contact:
George Stephanopoulos (Task Force Chair)
MIT, Department of Chemical Engineering
Room 66-562
Cambridge, MA 02139
or
Jim Davis
Department of Chemical Engineering
Ohio State University
140 West 19th Ave.
Columbus, Ohio 43210

Douglas J. Cooper is currently assistant professor of chemical engineering at the University of Connecticut, received his Ph.D. in chemical engineering from the University of Colorado in 1985. Prior to that, Dr. Cooper worked for three years in the Computer Process Control Division at Chevron Research Company in Richmond, Ca. His research at the University of Connecticut is organized under the auspices of the Laboratory for Intelligent Process Systems, of which he is Lab Director. His research focuses on using expert systems and neural networks for the automated design, implementation and adaptation of process control strategies. He also directs an experimental program studying the icineration of hazardous wastes using a circulating fluidized bed incinerator. Dr. Cooper's teaching specialties, both at the undergraduate and graduate level. include process control and numerical analysis.

Richard Mah is currently Professor of Chemical Engineeering at Northwestern University. He received his B.Sc. from the University of Birmingham and his Ph.D. from the University of London (Imperial College). Before joining the faculty at Northwestern University in 1972, he worked in industry for about 10 years, including 4 years as a group head at Esso Mathematics and Systems. He is a founding member of the AIChE CAST Division and a past chairman of its Programming Board. For his many contributions to computer-aided process design, he was named the recipient of the AIChE Computing in Chemical Engineering Award. He also received the Yack Youden Prize of the American Society for Quality Control. He has served in a variety of capacities with CACHE since 1972, including President (1984-86), Vice-President (1982-84). Computer Graphics Task Force, Secretary and Trustee. He is currently Chairman of the Conferences Standing Committee



Jeffrey C. Kantor is currently an Associate Professor of Chemical Engineering at the University of Notre Dame. He joined Notre Dame in 1981 after obtaining a Ph.D. from Princeton University and a one-year research appointment at the University of Tel Aviv. Professor Kantor's research interests are in process control focusing on nonlinear geometric methods, synthesis of multivariable linear controls for systems with hard constraints, and the control of discrete-event systems. It is the last research interest which occasionally causes him to encounter techniques developed in the AI arena.

Purdue-Industry ChE Laboratory Modules

R. G. Squires. G. V Reklaitis. M. Yeh
School of Chemical Engineering
Purdue University

P. K. Andersen
Department of Freshman Engineering
Purdue University

At Purdue, we are developing a series of computer simulations intended for use in undergraduate chemical engineering laboratories. These simulations are unusual in that they closely model the operation of actual industrial chemical processes. They are being produced with the assistance of various corporate sponsors (Table 1). Each sponsor provides detailed information on operating costs, flow rates, temperatures, pressures, and so on. The companies also produce a 20-minute video tape showing the actual plant that is being simulated.

Table 1—Modules and Industrial Sponsors

Company	Module
Amoco Oil	Hydrodefulfurization
Mobil	Catalytic Reforming
Tennessee Eastman	Methyl Acetate from Coal
Dow Chemical	Latex Emulsion Polymerization
Air Products	Process Heat Transfer

Amoco Hydrodesulfurization Module

We have completed one laboratory module, simulating a hydrodesulfurization pilot plant built by Amoco in their Naperville research facility. This module has been used successfully for the past two years at Purdue, and is currently being evaluated by several other schools (Connecticut, Georgia Tech, Michigan, North Carolina State, and Northwestern.

The Amoco program can simulate the steady-state operation of a small (0.12 ft3 laboratory reactor, and as many as three pilot plant reactors (12 ft3 each) in series. It also simulates the unsteady-state performance of a single pilot plant reactor.

The program has a convenient graphical user interface, and makes extensive use of a mouse. Using the mouse, the student can select an operating mode, request a printout, get on-screen help, or quit the program.

Figure 1 shows the screen that appears when the LABORATORY option is selected. It shows a schematic of the laboratory reactor, and another menu bar. Selecting INPUT on this menu brings up a box for the feed composition, flow rates, as shown in Figure 2.

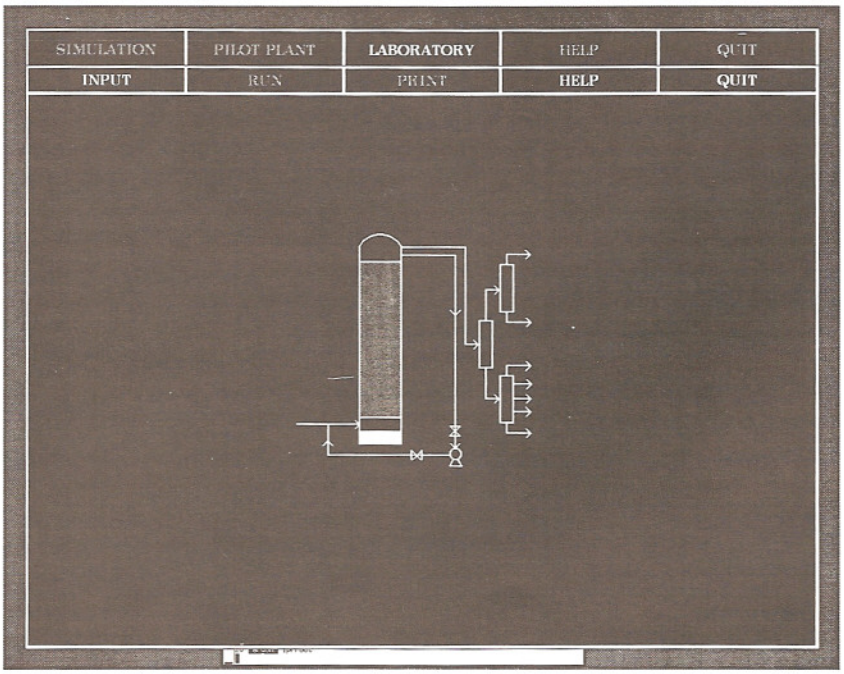


Figure #1

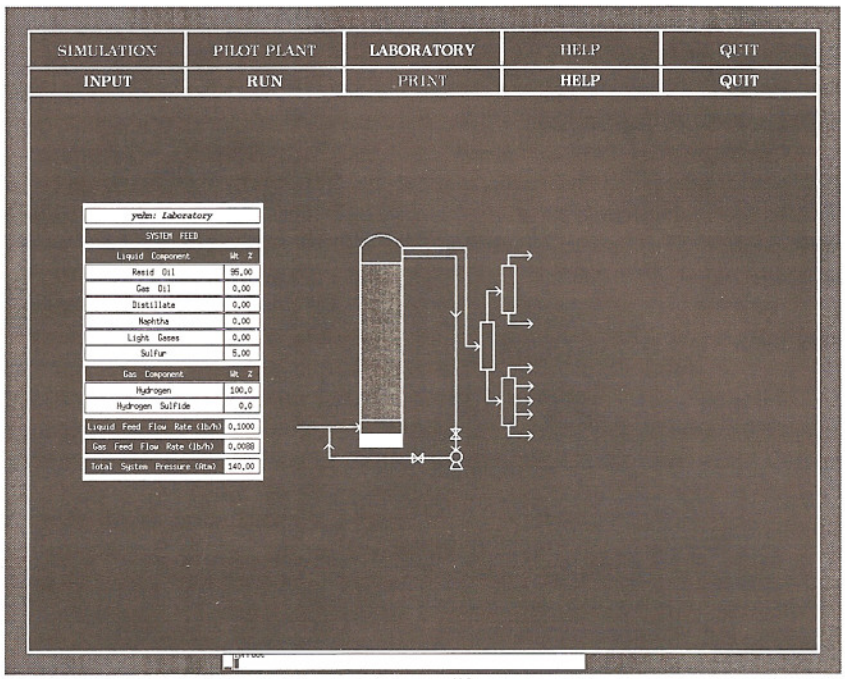


Figure #2

Once the required data are supplied, the student may run the simulation. The results are displayed on the screen Figure 3.

Using the Module

Our chemical engineering laboratory course (CHE 435) is held in two three-hour sessions each week. Students work in groups of three, consisting of a group leader, an experimentalist, and a design engineer. Each group works on three projects, one of which may be a computer simulation.

Before the first lab period, the students are given a memo-written on Amoco letterhead-which describes the problem they are to solve and the resources available to them, including the "budget" (simulated, of course) they have to work with. They are required to view a video "plant tour" of the actual Amoco facility, and to

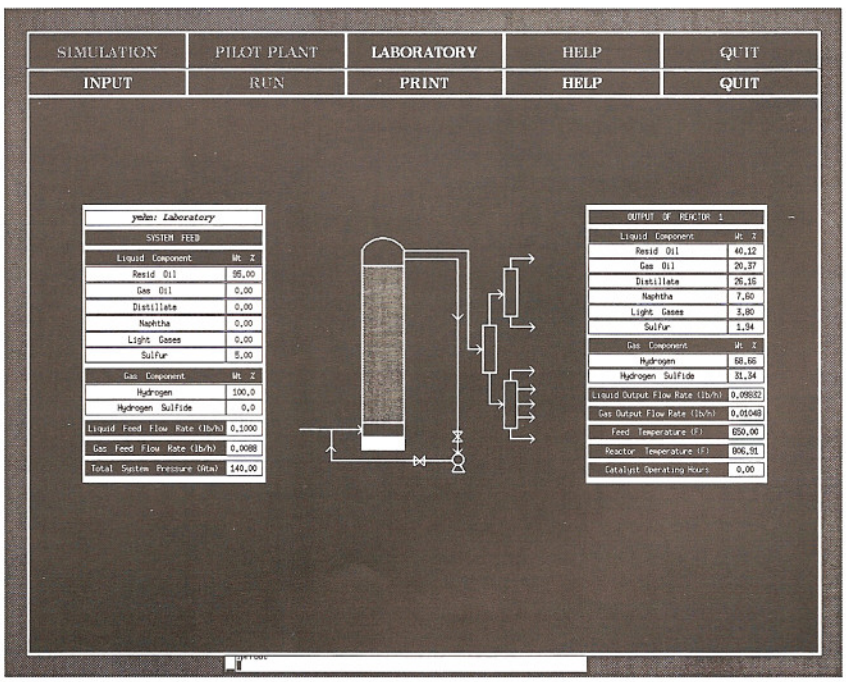


Figure #3

attend an orientation meeting.

Eight lab periods are allotted to each project. The first two periods are spent preparing a plan of attack, which must be presented to the instructor in a Planning Conference before the third period. Students may take data from the second through the sixth lab period. During the sixth period, the leader is required to give a 15-minute oral progress report, and a full written report is due one week after the last (eighth) period.

Budget and Expenses

The need to work within budget constraints adds considerably to the realism of the simulation. For the Amoco project, the students are given a simulated budget of $150,000. A list of expenses is shown in Table 2. Note that the initial plant start-up consumes half of this, leaving $75,000. Laboratory runs cost $500 each, pilot plant runs as $4,000 each. (Weekend runs cost more.) Students can request the help of a "consultant" (the instructor) who charges $500 a visit.

Table 2—Expenses

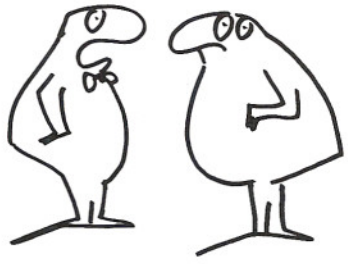
Initial preparation & start-up of pilot plant (includes cost of initial charge of catalyst)	5 days	$75,000
Replacement of catalyst in pilot plant	3 days	$50,000
One pilot plant run (includes labor, materials, analysis, etc.)		
3 reactors in series	24 hours	$4,500*
2 reactors in series	24 hours	$4,000*
1 reactor	24 hours	$3,500*
One laboratory reactor run (includes catalyst replacement)	24 hours	$500*
Consultation	?	$500

**Multiply by 1.5 for Saturday runs, by 2.0 for Sunday runs.*

Hardware and Portability

The modules are written in C, and make use of X-windows under the UNIX operating system. Some of the modules also use IMSL FORTRAN routines. At Purdue, the modules are being written for Sun workstations. However, given the portability of C programs, as well as the widespread availability of UNIX and X-Windows, it should be possible to run the modules on other machines with little or no modification.

Acknowledgements...
This program is supported by the National Science Foundation (Grant No. USE-8854614), Amoco Chemicals Corporation, Dow Chemical Company, Mobil Corporation, Tennessee Eastman Corporation, and Air Products and Chemicals, Inc. Completed modules will be distributed through the CACHE Corporation.



"Anything can be made to work if you fiddle with it long enough."

Example of Shareware: The MBT Master Directory Listing

Peter Rony, Virginia Tech

"The MBT" is a local shareware file server that serves both the university and the town communities in Blacksburg, Virginia. It has over 4500 files on line, with a total of 210 megabytes of storage. Several months ago, a student at the university brought The MBT Master Directory Listing to my attention; I was surprised to see how extensive it was. The directory headings are printed below to illustrate the types of software available. Similar shareware file servers should exist in most major cities.

Directory #1. IBM Compatible Screen/Keyboard/Mouse/Printer Utilities
- IBM Screen Utils
- IBM Keyboard Utils
- IBM Printer Utils
- IBM Mouse Utils

Directory #2. IBM Compatible Disk/RAMdisk/File Utilities
- IBM Disk Utils
- IBM RAMdisk Utils
- IBM File Utils

Directory #3. IBM Programming Utilities (MS DOS Programming)
- APL
- Assembler
- BASIC
  - C
  - Forth
  - Fortran
  - LISP
  - Pascal
  - Prolog
  - Other

Directory #4. IBM Editor/Word Processing/DBMS/Spreadsheet
- Text Processing
- DBMS
- Spreadsheeting
- Miscellaneous

Directory #5. IBM DOS Utilities
- DOS Utilities
  - BATCH Utilities
  - Equipment/Speed
  - Memory Utilities
  - DOS Shells
  - OS 2
  - Windows
  - Networks

Directory #6. IBM General Utilities
- MS DOS Utilities

Directory #7. Communication
- IBM Communications

Directory #8. Files for New Users
- New User Files
- *Of Interest to SYSOPS Only*

Directory #9. Turbo Pascal
- Turbo Pascal
- Turbo Pascal 4.0
- TSHELL

Directory #10 (Not in use)

Directory #11. Text Files
- Text Files

Directory #12 (Not in use)

Directory#13. Technical Discussion
- Processors
  - Drives/Controllers
  - Diagnostics
  - Languages
  - DOS
  - Keyboards

Multitasking
Memory Resident
Memory
Misc

Directory #14.
Technical Programs
Programs

Directors #15-#19 (Not in use)

Directory #20. Recent Uploads
(Have not been reviewed by the SYSOP)

Directory #21. MS-DOS Arcade Games

Directory #22. MS-DOS Strategy Games

Directory #23. MS-DOS Adventure Games

Directory #24. MS-DOS Music Programs

Directory #25. MS-DOS Games Over a Modem

Directory #26. MS-DOS Games Requiring EGA or VGA

Directory #27. Expansions for Commercial Games

Directory #28. MS-DOS Miscellaneous Entertainment

Directory #29. Games — Recent Uploads

Graphics Directory #21. ReadMac (Graphics Picture Display)

Graphics Directory #22. GIF

Graphics Directory #23. PrintMaster/PrintShop

Graphics Directory #24. ANSI

Graphics Directory #25. Viewers (ReadMac, GIF, Misc.)

Graphics Directory #26. Editors (MAC, GIF, Misc.)

Graphics Directory #27 (Not used)

Graphics Directory #28. Misc

MMM Directory #21. Publishing Printer Utilities
Laser Printer Fonts
Printer Utilities

MMM Directory #21. Other Utilities for Publishing

Graphics Utilities
System Utilities

MMM Directory #22. Publishing Text Files

Publishing Text Files

MMMMM Directory #21. PCBoard Utilities and DOORS

MMMMM Directory #22. Files for Various BBS Systems

MMMMM Directory #23. SYSOPS Recent Uploads

Directory 21. AMIGA Utilities

Directory 22. AMIGA Sight and Sound

Directory 23. AMIGA Games

Directory 24. AMIGA Text Files

Directory 25. AMIGA Programming Languages and Source Files

Directory 26. Recent AMIGA Uploads

SIMUSOLV*, A New Code For Modeling and Optimization

C.J. Burt
Central Research, Dow Chemical Company

What is *SimuSolv*?

The ***SimuSolv**** COMPUTER PROGRAM is an integrated, multifunctional software package designed to help scientists and engineers develop and use mathematical models of physical systems. It allows them to **simulate** the behavior of systems, to **optimize** performance, and to estimate the best values for model parameters. The program was developed within The Dow Chemical Company by professional modelers to increase their own productivity and to encourage researchers without extensive computer experience to avail themselves of the power of computer-aided modeling techniques. As a result, ***SimuSolv*** is very user friendly. Its philosophy is to provide maximal efficiency in problem-solving with minimal involvement in computational procedures. To this end, ***SimuSolv*** employs the powerful, high-level Advanced Continuous Simulation Language ACSL**. The language enables persons with limited programming experience to develop complicated models consisting of algebraic and differential equations, but still allows skilled programmers full rein to develop special applications utilizing MACROs, FORTRAN subroutines and sophisticated programming techniques. In addition, ***SimuSolv*** supplies extensive graphics, optimization, and simulation capabilities which are made easy to use by having almost intuitive basic commands along with defaults for most auxiliary commands. Versatility is maintained by providing almost complete control of these capabilities as required.

SimuSolv has been used extensively during its evolution to solve modeling problems in such diverse fields as process engineering, toxicology, pharmacology, chemical kinetics, environmental sciences, and agriculture. This practical experience has provided a wealth of expertise in the use of the package as well as in modeling techniques themselves. This expertise may be tapped by users of ***SimuSolv*** through the hot-line support provided.

History of *SimuSolv*

In the late 1960s and early 1970, scientists and engineers at The Dow Chemical Company were using digital computers in their modeling activities. Packages, such as Advanced Continuous Simulation Language (ACSL®, Mitchell and Gauthier Associates, Inc. of Concord, Massachusetts), were available for simulation and were easy to use, but they didn't contain algorithms for fitting nonlinear models to experimental data. Other packages, such as BARD (an IBM contributed program), provided parameter estimation but required advanced programming skills.

By 1978, the Computations Research Lab agreed that a software package that performed simulations as well as the "fitting" of experimental data should be developed. The envisioned product was to be easy to use. Its use should require only a minimal working knowledge of calculus, nonlinear parameter estimation techniques, optimization theory and computer science. After lengthy study, ACSL was chosen as the best foundation for building a package that would meet these requirements.

Over the next two years, ACSL was enhanced to include commands to bring in experimental data, to estimate and optimize model parameters, and to provide on-line help information. Moreover, the parameter estimation algorithm (which uses the Method of Maximum Likelihood) was modified to include an error model. This error models measures the nonhomogeneity of the variability in the experimental measurements —a feature desired by many statisticians. Procedures for general, nonlinear, constrained optimization were also added. The result was DACSL (Dow Advanced Continuous Simulation Language). DACSL was made available throughout Dow for use in classes .

Five years later, a small group was formed in the Engineering Research Laboratory in Central Research. This group was to test DACSL, now known by the trademark ***SimuSolv***, on the open market. In preparation, the package was generalized and enhanced by improving the parameter estimation routines, adding graphical interfaces for more devices, and making it compatible with different computer architectures.

In 1986 ***SimuSolv*** was beta-tested at a number of governmental and industrial sites. The interest generated by these tests, as well as the continued use of ***SimuSolv*** within Dow, confirmed the belief that there was indeed a market for the program. This led to the selection of distributors for ***SimuSolv*** in the United States and Europe.

Currently, work is in progress to upgrade ***SimuSolv*** , to V2.0, which should be completed late this year. Some of the modifications and additions include an extensively revised REFERENCE GUIDE, the Livermore Solver for Ordinary Differential Equations (LSODE), double precision numerical integration algorithms, the Direct Decoupled Method for sensitivity analysis, and two additional optimization algorithms.

The use of the ***SimuSolv*** computer program is continuing to grow. Many licenses have been granted to corporations, government agencies and universities throughout the world. And the program is being utilized in a variety of fields including process engineering, toxicology, pharmacology, chemical kinetics, environmental sciences and agriculture where its simulation, parameter estimation and optimization abilities are proving to be increasingly to be increasingly valuable. The technical support group is also growing to meet the needs of new users while continuing to enhance the capabilities of ***SimuSolv***.

What *SimuSolv* Can Do

• ESTIMATE PARAMETERS

Once you have put the mathematical model into an ACSL program, ***SimuSolv*** can be used to estimate unknown parameters. You can choose an optimization method or you can let ***SimuSolv*** choose the method. For small problems, ***SimuSolv*** chooses the Nelder-Mead simplex direct-search strategy, and for larger problems, a well-tested implementation of the generalized reduced gradient method. Simultaneous estimation of the parameters in an experimental error model and in the physical model ensures proper weighting of the data. The reported results give quantitative criteria for testing model adequacy along with the uncertainty of the estimated values. They also provide enough statistical information to enable you to choose the best model from several candidates.

• OPTIMIZE SYSTEMS

The parameter estimation capability of ***SimuSolv*** is just one application of its optimization techniques. During the estimation, ***SimuSolv*** maximizes the likelihood function which is a measure of how well the model fits the experimental data. But suppose you had a model of a process for making a chemical or drug, and part of the model defined how much profit the plan was making. Naturally, you would want to determine the operating conditions which maximize your profits. You can do that with the help of ***SimuSolv*** by defining profit as the criterion for the optimization and using the critical operating conditions as the adjustable parameters. ***SimuSolv*** can then systematically vary the parameters until the criterion is maximized.

SimuSolv features optimization methods which effectively handle such feasibility constraints.

• AUTOMATE DATA ANALYSIS

The ability of ***SimuSolv*** to incorporate FORTRAN subroutines and to use the MACRO features of ACSL enables it to be tailored for special applications. Such tailoring requires programming expertise, but the results can be highly beneficial.

Suppose you are studying the fate of various chemicals in the environment. You have set up a series of laboratory experiments and you will be doing extensive analytical work to determine time-concentration profiles. The data will need to be analyzed to determine rate parameters and to choose the best of several predefined models. The data storage and analysis could be automated using MACROs and FORTRAN subroutines designed to provide the following:

- A form for entering the conditions of each experiment, such as the name of the chemical, the dosage, the temperature, and so on.
- A form for entering the time and analytical results for each observation.
- A menu to allow the researcher to

— ask ***SimuSolv*** to find the best set of rate constants to fit each type of model to the date.

— display or print a graph of calculated curve alongwith the experimental points.

— display or print a table of the predicted and experimental results, along with goodness-of-fit statistics, and

— print out a standard report.

With this type of automation, the lab workers would need to know only a modicum about computers and data analysis methods, and could concentrate their time and thoughts on their studies rather than on the mechanics of using the computer.

• SIMULATE PHYSICAL SYSTEMS

Let's assume that you have available a mathematical model of a physical system of interest to you. You wish to study the model and to predict the behaviour of the system. To do this you will have to translate the model into a computer program and ask the computer to run the program (i.e., integrate the equations) and show

you the results as a graph or a table of values. The ***SimuSolv*** computer program allows you to use the ACSL language to write the program and enter the values of all the parameters. With very simple commands ***SimuSolv*** will run the program and show you the results.

Numerical integration of differential equations can require large amounts of computer time. It is important, therefore, to choose an integration method which will efficiently solve the type of equations in your model. ***SimuSolv*** provides several methods to select from so that you can minimize the amount of computer time (and costs) required to solve your problem. These methods range from the simple Euler routine to state-of-the-art techniques such as the Livermore Solver for Ordinary Differential Equations (LSODE) for stiff systems of equations.

You can:

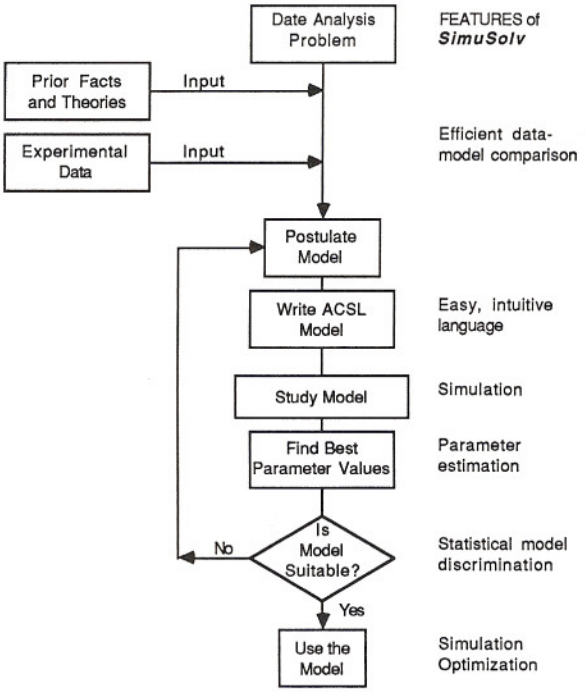
- display graphs of calculated results and compare experimental data with calculated curves
- change the value of parameters
- label and print out tables of values
- ask "What if?" questions to obtain an intuitive feel for the characteristics of the model
- test the sensitivity of your system to changes in conditions
- change the integration method to improve computational efficiency.
- Develop Mathematical Models

Developing mathematical models of physical systems is a fundamental part of the scientific method. It is an iterative process as you can see in the accompanying flow sheet. Data are collected, hypotheses are proposed to correlate and explain the data, and hypotheses are tested. When necessary, more data are collected. When the hypotheses are in conflict with data, they are modified.

The simulation, parameter estimation and statistical capabilities of ***SimuSolv*** can help you in each step of this iterative process. (*see graph at top right*)

Although many problems solved by ***SimuSolv*** involve the integration of differential equations, this example program illustrates how ***SimuSolv*** can be used to fit model equations to data when the model is a set of nonlinear equations. A model definition program structurally identical to this one was used to test reaction rate expressions, and to fit the kinetic parameters, with data collected during the steady state operation of a Berty

MODEL BUILDING WITH *SimuSolv*



Example of Steady State Reactor Modeling

reactor which is a CSTR (continuous stirred tank reactor).

The proposed physical system for this single reversible gas phase reaction can be described as

$$A + 2B \;<==>\; C + D$$

This can be written, mathematically, as:

$$\text{Rate} = k_1 P_A P_B^{\,m} - k_2 P_C P_D$$

$$= k_1 P_A P_B^{\,m} \left(1 - \frac{k_2 P_C P_D}{k_1 P_A P_B^{\,m}}\right)$$

$$\text{Since KE} = \frac{k_1}{k_2}$$

$$\text{Rate} = k_1 P_A P_B^{\,m} \left(1 - \frac{P_C P_D}{KE\, P_A P_B^{\,m}}\right)$$

where m = ORDER.

The proposed model for the reaction rate equation is written in terms of the component partial pressures (PA, PB, PC, and PD), the unknown kinetic parameters (K, the rate constant, and KE, the equilibrium constant) and the B component reaction order (ORDER). The rate of reaction of component A is also directly calculated from the conversion of A (X), feed rate of A (Feed), and reactor volume (Volume). The partial pressures are calculated from known experimental parameters and X.

For each set of data, two rates of reaction are determined—one from the proposed model and one from direct calculation. The difference between these two should be negligible if the model is correct.

For each pass through the dynamic segment, a line of data must be brought into the model program for use in the equations. Each pass is controlled by the CINT variable and the run variable, N. N, which is assigned an initial value of 1 in order to correspond to the first line of data, is incremented by CINT, whose value is also 1, until the termination condition (found in the TERMT statement) is met.

With CINT and N both equal to 1, the run variable becomes a counter that can be matched to the lines of data. The LINEAR function, encountered with each pass through the dynamic segment, reads in the corresponding data line. The looping stops when the run variable, N, becomes greater than or equal to Ntotal, the total number of data sets. In this way, during a given program run, all the data are brought in with calculations made on each set.

The data include a dummy variable, Error, which is set to zero for all sets. Error is used as the fit variable for an optimization command when fitting the model parameters with the data. Error is the difference between the experimentally determined rate (Rate) and the model rate (RateP). An identical variable, Resid, is given the same value as Error, because the plots of Error give the data points (i.e., 0.0s). Resid will have the true difference between the two rates.

The run-time command file contains all the commands and data to do the parameter estimation of K and KE and the fitting of the calculated Error (FIT Error ...) to its data counterpart, which is 0.0 for all data sets, while keeping the heteroscedasticity parameter parameter set to 0 (... = 0). All sequences of commands that are to be repeated are written in PROCs. One PROC, called doit, will do the parameter estimation. Other PROCs handle the plot commands. The data set is included in a PROC as well. If there were more than one set of data each inside a separate PROC, then each could be used when desired by naming the PROC.

The last 22 lines of the file give the commands necessary to test the models and produce the graphs. First, the data are brought into the model. The order of the B component is set. The parameters are calculated. The plots are displayed. Then the order is changed, and the above process is repeated.

The reports giving the value of the Maximum Likelihood function show that the model with Order=2 (MLL=20.039) provides a better fit than with Order=l (MLL = -l05.42).

The plot of RateP versus Rate gives a good visualization of the overall goodness of fit. Plots of Resid versus the experimental parameters (Feed, T, Ptotal, BtoA and ltoA) are used to see if the error is random. If it isn't, then a better model should be sought.

Course Available

A course entitled "An introduction to ***SimuSolv***" is available for users of ***SimuSolv***. The course covers all the basics, from the simple mechanics of invoking ***SimuSolv*** to the creation and utilization of complex model definition programs. A choice of problem sets is available: one focusing on biological/pharmacokinetic applications, the other on chemistry/chemical engineering applications. The course is in the form of a workshop with significant time spent on the computer. It is taught at the user's location by members of the Dow technical staff.

For further information, call (517) 636-1879.

Documentation Available

A second printing of the *INTRODUCTORY GUIDE To SimuSolv* by E.C. Steiner, G.E. Blau and G. L. Agin is now available through the distributors. Cost is $15.00.

Distributors:

Mitchell and Gauthier Assoc., Inc.
73 Junction Square Drive
Concord, Massachusetts 01742
Telephone: (508) 369-5115
Telex: 951 572

Rapid Data, Ltd.
Crescent House
Crescent Road
Worthing
West Sussex BN111 5RW, England
Telephone: (0903) 202819
Telex: 87661 RADATA G

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** Registered Trademark of Mitchell and Gauthier Associates, Inc.

Electronic Mail Task Force

Peter R. Rony, Virginia Tech

AIChE New York Headquarters is on BITNET

May 26, 1989 may well go down as an important date in the annals of the AIChE. On that day a small step for AIChE-kind occurred: Ralph Mordo, who is director of computer operations at AIChE headquarters in New York, successfully sent the first AIChE messages over BITNET. Ralph's BITNET userid is CHEAIS at CCNYVME.

AIChE headquarters will, in time, represent the leading edge of attempts to use email to interconnect key segments of the membership of AIChE (e.g., all chemical engineering departments, the meeting program chairman and session chairman, local AIChE chapters, and so forth). The next opportunity for the Electronic Mail Task Force is for us to involve and assist AIChE in some test that involves required and useful communications between headquarters and selected academic faculty.

AIChE Journal is a User of BITNET

Morton Denn (denn@violet. berkeley.edu) sent an electronic mail message that stated the following: "AIChE Journal has for a number of months had an e-mail address (aichej @violet. berkeley. edu) which appears on our letterhead. We encourage authors and reviewers to use e-mail (though few do). We will not accept electronically transmitted manuscripts, however, because then we would have to produce hard copy for the reviewers and editorial staff."

Clearly, AIChE Journal leads the AIChE in the use of electronic mail within the Institute.

Validation of BITNET Userids

The Electronic Mail Task Force has been in the process of validating its nickname userid list. The current version is dated June 3, 1989. This new, 45-page list has been subdivided into two parts, one for verified userids and a second for non-verified userids. To get an electronic copy of this updated list, send a request over BITNET to RONY at VTVM1. Ask for the following file:

RONY NAMES A0,
Current version of IBM mainframe nickname file for ChE BITNET userids, June 6, 1989

which can be used immediately on all IBM mainframes.

Robert Brodkey (brodkey at kcgll.eng.ohio-state.edu), a contributor to the Spring 1989 CACHE News, has been added to the task force. Bob has been converting an earlier version of the updated IBM nickname listing to a VAX nickname listing, a valuable and appreciated service. As a consequence of Bob's input, it will be easier for a database program to manipulate each userid set of entries. This change will facilitate the creation of specialized lists (e.g., userids alphabetized by name). For example, in the next version of the RONY NAMES A0 list, the University name will appear first, immediately after the keyword, address:

address.Illinois, University of

Bob's VAX files are available from the Task Force database in Blacksburg. Send a request to RONY at VTVM1, and ask for BRODKEY FILES A0, which contains the following files:

MAIL_NAMES.CHE
A coded listing that is kept on the VAX public disk in the form of a file called MAIL_ALIAS.DAT

NICKNAME.VER
A verified listing of the nicknames. This list does not contain any unverified name.

Bob writes:
"An aliasing facility has been added to MAIL [on a VAX] that allows you to specify destination addresses by a short 'nickname' string rather than a long network address. A list of nicknames for chemical engineering professors has been generated for you to use. The list, comes from CACHE and adapted for a VAX, was compiled by Peter Rony. To make the CACHE list available for use in mail on a VAX, you must add the following lines to your LOGIN.COM file:

$define mail_alias_files -
sys$login:mail_alias.dat,

common$disk:[ce.mail]mail_alias.dat

"To actually use the facility from inside of MAIL, specify the destination address for a SEND or MAIL command as follows:

alias%"nickname"

where 'nickname' is the nickname for the person to whom you are sending the electronic mail. Note that the percent sign (%) and double quote marks (") must be specified.

"In addition to the pre-defined CACHE nicknames, you can define your own nicknames by creating a mail_alias.dat file in your login directory. Each line of the mail_alias.dat file defines one nickname and has the format:

nickname : email-address

Type

COMMON$DISK:[CE.MAIL]MAIL
_ALIAS.DAT

for examples.

"We will keep the public department listing up to date. Note also that it can take several seconds to fully search the nickname file. There are over 500 people and universities on the list.

"Finally, if you find any errors, send a message to BRODKEY. For our local VAX account at Ohio State, we do not need to use the alias procedure; thus, the name will be adequate."

Chemical Engineering Email Bulletin Boards and Services

A message from a member of the email task force, John Hassler (University of Maine), who has given permission to repeat his comments, appraises the current situation:

"Has there been any activity at all on either of the ChE bulletin boards? I haven't heard of any. Our computer center just started getting the feed from UUNET. There is lots of activity there; I don't see why ChE doesn't have an active BB.

"UUNET: Unix Users Net, sometimes known also as USENET, was probably the second nationwide network (after Arpanet). It just sort of "grew", and is relatively unstructured (read "anarchic"). The "netnews" bulletin board is a collection of a couple of hundred topics that people all over the world contribute to. Our computer center director describes it as "an information junkie's dream". I am, and it is. Presently, for example, I am closely following the "cold fusion" discussion, one on "computer architecture", one on "C language", one on "numerical methods", etc., and I occasionally look at many others. When we first got it here, I was spending over an hour a day just reading the news. I've had to limit myself, but I may spend a couple of hours today (Saturday) catching up on things.

"We have it on our mainframe as NETNEWS. I just type NETNEWS, and it sets up the reader program. If you have it, you might try that, or HELP NETNEWS, or HELP MENU NETNEWS, or something. I know that VPI has access, because I have seen postings from there, but I don't remember whether they came through the computing center, or from some particular lab's VAX. (The original UUNET was set up by people using UNIX on

DEC PDP-11's, and it still seems to be strongly oriented that way, though a lot of mainframes have gateways now.)

"According to our computer center, NETNEWS costs nothing except the telephone line connect time, so you may have access to it one way or another. If you have trouble finding it, I'll watch for somebody from VPI posting a message, and give you his name. As I mentioned, UUNET is so very active in all sorts of fields of interest that it surprises me not to see this type of activity on the two ChE BB's that have been set up. Don't ChE types have anything to discuss?"

BITNET Discussion Group: Interfacial Phenomena

The task force recently has received, from Bill Plymale at Virginia Tech, a printed copy of the LISTSERV GROUPS (version 04/06/89), which identifies BITNET discussion groups. Many, if not most, are of no interest to chemical engineering faculty, but the following discussion group based at Washington State University should be noted:

List: IFPHEN-L at WSUVM1
Coordinator: Richard L. Zollars (SCEF0002 at WSUVM1)
Interfacial Phenomena Interest List: A discussion group on Interfacial Phenomena (Group 1c, American Institute of Chemical Engineers).
Includes meetings, articles, software, theories, materials, methods, tools, etc.

Distributing Mathematical Software Via Electronic Mail

Jack Dongarra,Eric Grosse
Argonne National Laboratory

A quick, easy, inexpensive way to get public-domain software electronically

Engineers and scientists throughout the world are using collections of high-quality mathematical software at universities and in industry. Typically, this software is obtained from distribution agents—for example, IMSL, the National Energy Software Center (NESC), and the Numerical Algorithms Group (NAG). All these agencies do a fine job with the distribution of large packages of mathematical software. But how does one go about getting a single piece of software? The usual approach, unfortunately, entails sending a tape to an author, waiting until that author copies the program and mails back the tape, and then deciphering the often-alien tape format. The whole process can waste an intolerable amount of time.

We've developed a new system, called *netlib*, that provides quick, easy, and efficient distribution of public-domain software to the scientific computing community on an as-needed basis.

A user simply sends a request by electronic mail to *netlib@anl-mcs* on a national network such as ARPAnet, and receives the requested software over the network.

Netlib in use

Imagine an engineer who needs to compute several integrals numerically. He consults the resident numeric expert, who advises trying the routine *dqag* for some preliminary estimates and then using *gaussq* for the production runs. The engineer types at his terminal

mail research!netlib
send dqag from quadpack
send gaussq from go

In a short time, he receives back two pieces of mail from *netlibd*. The first contains the double-precision Fortran subroutine *dqag* and all the routines from *quadpack* and *dqag* calls; the second contains *gaussq* and the routines it calls.

Should the engineer later decide that the routine *dqags* would be more effective, he could ask send *dqags* but not *dqag* from *quadpack* to get *dqags* and any subroutines not already sent with *dqag*.

This engineer happens to be connected to the UNIX network. If, instead, his machine was on the ARPAnet, he would use the address *netlib@anl-mcs*. If he needed the code in upper case, he would send his request in all caps; to get single precision, he need simply change the names of the routines or the libraries as appropriate.

As typical examples we give the following (with an explanation in parentheses):

send dgeco from linpack
(Retrieves routine DGECO and all routines it calls from the LINPACK library.)

send only dgeco from linpack
(Retrieves just DGECO and not subsidiary routines.)

send dgeco but not dgefa from linpack
(Retrieves DGECO and subsidiaries, but excludes DGEFA and subsidiaries.)

send list of dgeco from linpack
(Retrieves just the file names rather than the content; this can be helpful when one already has an entire library and just wants to know what pieces are needed in a particular application.)

find eigenvalue
(Retrieves the names of routines in the collection related to the keyword *eigenvalue*.)

whois france
(Retrieves all addresses of people in the database living in France.)

Netlib tolerates minor syntax deviations, since we do get requests like "Please send me rlmach from port. Thank you." Apparently, the system is so easy to use that people don't realize they're talking to a program. One user even sent "sned index 4 eispack" instead of "send index for eispack" so we've made "4" a synonym for "for" and "from." However, we make no attempt to accept arbitrary English—or any other language.

Quick response

Just how quickly requests are answered depends on the speed of the network communications involved. Five or ten minutes is typical for ARPAnet, while UNIX uucp may require anywhere from minutes to days.

The actual processing time is insignificant. One user wrote back enthusiastically that the system was so fast he preferred using it to hunting around on his own machine for the library software.

The heart of the collection

Table 1 lists the public-domain software currently included in *netlib*. But the real heart of the collection lies in the recent research codes and the "golden oldies" that somehow never made it into standard libraries. Almost all of these programs are in Fortran, although some are in C (such as the routine *rainbow* for generating uniformly spaced colors. There are also descriptions and benchmark data for various computers, a collection of errata for numerical books, test data for linear programming collected by Gay, and the "na-list" electronic address book maintained by G. Golub.

In addition, we have included a few odds and ends for convenience, such as technical memoranda and reports produced by the Mathematics and Computer Science Division at Argonne.

We do *not* send out entire libraries. A computer center setting up a comprehensive numerical library should get magnetic tapes though the usual channels.

Security and other problems

Might not someone tamper with the program text as it is en route to the user? Yes, that is of course possible, but for the moment we feel that the threat is minimal. If this situation changes, we can easily adopt encryption schemes.

We have encountered problems occasionally with computers that are willing to send us mail but will not allow us to send mail back. Delays for multihop and internetwork mail are more common, but we have no way to collect statistics on these, and in any event such delays are out of our control.

The most difficult problem we have encountered has been length limitation; a few of the programs are more than 100 kilobytes, and that is more than the mail systems at many ARPAnet sites will tolerate. We did consider using Huffman coding to compress the files, but that would save only about a factor of two and would require that we ship decoding programs. Instead, we simply split up large items into several pieces of mail.

Comparison with other services

The *netlib* service provides its users with several important features:

- There are no administrative channels to go through.
- Since no human processes the request, it is possible to get software at any time, even in the middle of the night.
- The most up-to-date version is always available.
- Individual routines or pieces of a package can be obtained instead of a whole collection. (One of the problems with receiving a large package of software if the volume of material. Often only a few routines are required from a package, yet the material is distributed as a whole collection and cannot easily be stripped off.)
- It's free!

On the other hand, *netlib* is simply a clearinghouse for contributed software and therefore subject to various disadvantages that have plagued such projects in the past. The only documents, example programs, and implementation tests are those supplied by the code author or other users. Also, there may be multiple codes for the same task and no help in choosing which is best.

We have made an effort not to stock duplicate copies of machine constants, but in general we have left submitted codes untouched. We have also tried to be more selective than many personal computer bulletin board systems: we do not allow users to put their own software automatically in the collection. (This allows us some measure of control; we wish to avoid such problems as having our system confiscated because it contained a stolen telephone charge number.)

Promoting modern numerical techniques

Netlib cannot replace commercial software firms. We provide no consulting, make no claims for the quality of the software distributed, and do not even guarantee the service will continue (to date, we have received funding for the project from the National Science Foundation).

In compensation, the quick response time and the lack of bureaucratic, legal, and financial impediments encourage researchers to send us their codes. They know that their work can quickly be available to a wide audience for testing and use. We hope *netlib* will

promote the use of modern numerical techniques in general scientific computing.

Read more about it

J. J. Dongarra and E. Grosse, *Distribution of Mathematical Software via Electronic Mail*, Argonne National Laboratory Technical Memorandum MCS-TM-48 (March 1985)

About the author

Jack J. Dongarra is a Computer Scientist in the Mathematics and Computer Science Division, Argonne National Laboratory. He is also Scientific Director of the Advanced Computing Research Facility at Argonne and is actively engaged in linear algebra research.

Table One: Material Available through netlib

Package	Description
BENCHMARK	LINPACK and other timings.
BIHAR	Bjorstad's biharmonic solver.
BMP	Brent's multiple precision package.
CORE	Machine constants, Basic Linear Algebra Subprograms and extensions.
CALGO	Collected algorithms from ACM, published in Trans. Math. Soft.
CONFORMAL	Schwarz-Christoffel conformal mapping programs.
DOMINO	A parallel programming environment from the Univ. of Maryland.
EISPACK	Solution of eigenvalue problems.
ELEFUNT	Cody and Waite's tests for elementary functions.
ERRATA	Corrections to numerical books.
FISHPAK	Finite-difference approximately for elliptic BVP.
FITPAK	Cline's splines under tension.
FMM	Codes from book by Forsythe, Malcolm, and Moler.
FNLIB	Fullerton's special-function library.
FFTPACK	Swarztrauber's Fourier transforms.
HARWELL	MA28 Sparse matrix routine from the Harwell library.
HOMPACK	A continuation package.
ITPACK	Iterative linear-systems solvers.
LANCZOS	Cullum and Willoughby's Lanczos programs.
LASO	Scott's Lanczos program for eigenvalues of sparse matrices.
LINPACK	Solution of linear equations.
LP/DATA	Linear programming test data.
MACHINES	Short descriptions of various computers.
MICROSCOPE	Alfeld and Harris' system for discontinuity checking.
MINPAK	Nonlinear equations and least squares.
MINPACK	Optimization routines.
ODEPACK	Ordinary Differential Equations package.
PARANOIA	Kahan's test of floating point.
PCHIP	Hermite cubics by Fritsch and Carlson.
PLTMG	Bank's multigrid code; too large for ordinary mail.
PORT	The public subset of PORT library.
PPPACK	Spline routines from de Boor.
QUADPACK	Quadrature routines.
SIAM	Typesetting macros for SIAM journal format.
SLATEC	Machine constants and error handling package from the Slatec library.
SPECFUN	Transportable special functions.
TOPELITZ	Solution of systems of equations where the matrix is toeplitz.
Y12M	Package for sparse linear systems
miscellaneous	GAUSSQ, LOWESS, etc.

A User's Guide to Electronic Mail
(Part. 1)

Peter R. Rony, Virginia Tech

The Electronic Mail Task Force of CACHE has been responsible for promoting the use of electronic mail, particularly over the BITNET worldwide network, among chemical engineering educators. In addition to presentations at the fall national AIChE meeting, contributions to CACHE News, encouragement for the use of a BITNET wide-area network file server called GRAND, and maintenance of a BITNET nickname list for IBM mainframes, the task force also keeps on the lookout for tutorial information that would help the chemical engineering user community better understand the characteristics of electronic mail and networking. Dr. Bob Simon, of the National Research Council (Board on Chemical Sciences and Technology), brought a copy of the front matter from the AAS Electronic Mail Directory to our attention this past summer. As Bob stated, "I think it is particularly well done and am passing it along with the thought that AIChE might want to emulate it." We shall transmit this material first to chemical engineering educators whose institutions are members of CACHE. Permission has been granted by Peter Boyce, Executive Officer of the American Astronomical Society, for CACHE News to reproduce the first 18 pages of the following document. We have included cost and copyright details as well as the full text of a "Dear Colleague" message from Dr. Boyce. The message provides insight into the creation and validation of the email directory. Also observe that the AAS can communicate electronically usingnot just one but a variety of phone addresses and electronic network names: TELEX, FAX, TELEMAIL, ARPANET/INTERNET, and BITNET. The trustees of CACHE thank Dr. Boyce and the AAS for permission to reprint the following material in one or more issues of CACHE News. If you would like an electronic version of this material, and plan to use it only for non-commercial purposes, please contact RONY at VTVM1.

Peter Rony, Electronic Mail Task Force

American Astronomical Society
1989 Electronic Mail Directory

Published by:
American Astronomical Society
Executive Office
2000 Florida Avenue, NW
Suite 300
Washington, DC 20009

BITNET: aas at stsci
ARPANET/ITNERNET: aas at scivax.stsci.edu
SPAN: scivax::aas or 6549::aas
TELEMAIL: [pbouce/amerphys]telemail/usa
FAX: 202-234-2560
TELEX: 257 588 AASW UR

Address corrections for this Directory must be sent on the AAS Change of Address Card located in the back of the AAS 1989 Membership Directory. Additional copies for non-commercial usemust be purchased with the regular AAS 1989 Membership Directory and will not be sold separately. The cost a requests must be submitted in writing to the AAS Executive Office.

Dear Colleague:

This Directory of E-Mail addresses of AAAS Members has been compiled from responses to the form published in the AAS Newsletter. Of over 1200 E-mail addresses, we found serious errors with approximately 15 percent. Within the constraints of limited time, we have corrected obvious errors and, when the correction was not so obvious, we made phone and E-Mail inquiries to as many as possible of the 100 or so inadequate addresses. We have made no adjustments without testing the address or consulting the addressee. Clearly, it was impossible to test all addresses, so there will undoubtedly be errors. If you have trouble reaching an individual by E-Mail, please contact them by telephone. Please do not call the AAS Executive Office—all of our information is contained on the pages of this directory. The unanticipated high error rate and the difficulty of proofreading have delayed the publication of this Directory, for which we apologize.

A User's Guide to E-Mail has been included. We tried to make this helpful for uninitiated users. We would appreciate suggestions about how to improve

this directory. Please read the User's guide and use the tables at the end of the introduction to help you find the right format to use for connecting to foreign networks.

Where networks are not case-sensitive (see User's Guide), addresses are listed in lower case in order to save space. Addresses which are case sensitive have been published as they were sent in. We have give the "bare bones" address, leaving off such things as a trailing ".bitnet" or the quotation marks which some mailing software requires. These things are unique to each site and are not part of the address. Finally, be aware thatlong addresses have been split and carry on to a second line.

Finally, I want to thank Bob Hanisch of the Space Telescope Science Institute for his continuing help in organizing the development and production of the introduction and for answering our endless questions.

Peter B. Boyce
Executive Officer

Table of Network Abbreviations:

B	BITET/EARN/JANET
S	SPAN
I	INTERNET/ARPA/NSFNET
G	GTE TELEMAIL/NASAMAIL/ AURANET
U	UUCP
PSI	PSI
USE	USENET
M	MCI MAIL
X	TELEX

1. Introduction

Computer networks now span the world, and the gateways between them allow millions of users to send electronic mail messages to one another, permitting easy collaboration between researchers in different countries. However, the syntax required to send a message from one machine to another is often complicated, and there is no central register of electronic addresses for users. This directory is an attempt to provide ease of access to Society members via electronic means.

In order to send electronic mail it is typically necessary to know the user name of the addressee, the name of the machine on which he or she is working (the host), and the name of the network to which the machine is connected (the domain). This information may be obtained from the sender (Section 3 gives some hints on deciphering electronic mail addresses), or from this directory. Because there are several different networks in wide use, a lot of electronic mail has to cross from one network to another via gateway machines or relays. These are computers that are connected to two or more different networks and which accept mail from one network and forward it onto another network. Many of the mysteries of electronic mail have to do with determining the syntax needed to send mail through such relays. General advice on the syntax required to send electronic mail is given in Section 2. Information relating to specific networks may be found in Section 4. Users are warned that the information given in this guide cannot be guaranteed. In particular, the relay machines between the various networks tend to change, sometimes with little or no notice. We will endeavor to keep AAS members apprised of such changes through the AAS Newsletter and through the annual updates to this directory. This overview of electronic mail communications is drawn primarily from a document by Chris Benn and Ralph Martin of the Royal Greenwich Observatory, with editorial changes (to accommodate a North American point of view) and updates by Peter Shames and Bob Hanisch of the Space Telescope Science Institute and Peter Boyce of the AAS Executive Office.

2. Network Descriptions

The computer networks in most common use by astronomers in North America are the ARPA Internet, SPAN (NASA's Space Physics Analysis Network), BITNET, UUCP, and Telenet (a commercial network managed by GTE). In addition, astronomers worldwide have access to a number of other networks, such as JANET and Starlink in Britain, EARN in Europe, INFNET/ASTRONET in Italy, ACSNET in Australia, and the international packet-switched networks based on the X.25 protocol. Each of these networks will be described below. A number of other networks that may be encountered are mentioned in the Glossary.

Mail delivery times will vary from network to network; on SPAN mail delivery is essentially instantaneous (indeed, if the mail cannot be sent the user is informed of this immediately, and queuing of messages is not supported). On UUCP it may take several days for a message to reach its destination. Most networks provide mail delivery in times between a few minutes and a few hours, and if the mail does not go through immediately they will try again several times before returning the mail to the sender. Some networks only provide electronic mail services (such as BITNET and Telenet), while others allow users to log in on other computers and copy files (such as SPAN and INTERNET).

The current state of computer networks is some-

what akin to telephone systems around the turn of the century—there are numerous systems, some mutually incompatible, and some interconnected through gateways that provide mail forwarding services. Moreover, different networks use different protocols, or data encoding schemes, for the transmission of information. Some of these protocols are open standards, such as TCP/IP, and some are proprietary to certain manufacturers (such as DEC's DECnet). As a result, there is often no one simple way to specify a mail address. There is no equivalent to the standard telephone number, although there are "standard"' ways of specifying electronic mail addresses. This guide is intended to function like the front pages in your telephone book, which provide telephone dialing instructions, that most of us never read because it's all so simple and standardized. In the case of electronic mail, however, it is not simple and standardized and you do really need to read the "dialing instructions."

As far as the user is concerned, electronic mail/data communications lines are essentially error free; complex error checking and error correcting procedures are defined in the standards, and are carried out by a combination of hardware and software. As an alternative to data communications lines, one may use direct dial-up with normal telephone lines and error correcting modems. However, the costs compared with data communications networks are high over long distances, and the passband and signalling standards used on audio networks can vary from country to country, which may result in incompatibility between modems (e.g., between the USA and the UK). Generally, the costs of commercial data communications lines are related to the quantity of data transmitted, while direct dial-up costs are related to the length of time that a call takes. Different methods are used to encode the data on data communications lines and telephone lines. On telephone lines between modems, the data are encoded as a frequency modulated audio tone, and the transmission rate is limited by the bandwidth of the line, usually to 2400 baud (although baud rates up to 9600 can be obtained by using special modems). On data communications links, although the physical media may be similar, phase encoding is used which allows a much higher transmission rate, typically 9600 baud.

Standards for data communications links are defined by the International Standards Organization (ISO). ISO has attempted to identify a seven layer model describing the interconnection of computers of different types via any kind of network. The lower levels are concerned with hardware matters, such as defining the pin for the "transmit' line, while the upper layers are concerned with more esoteric problems, such as the means by which one might transmit an encrypted picture to a telex machine. However, there is still much confusion, because there exist competing standards from different organizations, such as TCP/IP from ARPA, DECNET from DEC, SNA from IBM and the "Coloured Book" protocols in the UK; some of which incorporate a mixture of ISO and proprietary protocols. The ISO standard protocols are still being developed, but when they are available many of these problems will diminish.

[NOTE on case sensitivity: Most electronic mail addresses are not case sensitive. Thus, throughout this directory you can usually equate an address such as user@site.domain with USER@SITE. DOMAIN. As a matter of convention the networks that are composed primarily of computers running the UNIX operating system tend to use lower case addresses (UUCP, INTERNET), and networks composed primarily of VMS machines use upper case addresses (SPAN). This is a tendency, however, not a strict rule. One should be careful with UUCP addresses in particular; users are advised to follow the case specifications carefully, since the address host1!host2!user is not the same as host1!host2!User. For more information about computer networks, readers are advised to refer to the excellent article "Notable Computer Networks" by J.S. Quarterman and J.C. Hoskins (Comm. A.C.M., 29, 932 (1986)).

ARPA INTERNET

The Defense Advanced Research Project Agency (D)ARPA network was initially set up by the U.S. Department of Defense in 1969. It is now a part of the ARPA INTERNET, which uses TCP/IP (Transmission Control Protocol/Internet Protocol) communications and includes over 30000 hosts (1987) and more than 570 networks in several domains:

COM	commercial organizations
EDU	educational/research organizations
GOV	civilian government organizations
MIL	Department of Defense
ORG	other organizations

Most INTERNET network sites that astronomers communicate with will be in the EDU domain (universities, national observatories). There are additional domains for countries outside the USA, e.g., UK (United Kingdom) and AU (Australia). INTERNET includes some transcontinental and transatlantic satellite links (SATNET). Typical delivery time on INTERNET is a few minutes.

In INTERNET individual computers are assigned numerical addresses within a hierarchical system, with the first number in the address being the number of the individual network on INTERNET. For example [4.0.0.0] is SATNET, [10.0.0.0] is the ARPA network, [128.112.0.0] is the Princeton network, and

[128.112.24.2] is an individual machine at Princeton. These addresses are mapped against alphanumeric addresses via host tables. Thus, the machine [128.112.24.2] corresponds to pupgg.princeton.edu. In fact, users will generally need to specify the alphanumeric name of the host, rather than its numerical address, when sending mail or doing a remote login. Other examples of INTERNET host names are stsci.edu, scivax.stsci.edu, noao.arizona.edu, and astro.umd.edu. These names all have at least two components (site.domain), and may have several fields separated by periods preceding the domain, e.g., astro.as.utexas.edu. These fields can generally be interpreted as a hierarchy machine, (subnet,) campus, domain.The Network Information Center (NIC) coordinates site and host numbers for all of the systems connected to INTERNET.

Additional information about INTERNET, including more detailed user's guides, can be obtained by logging in to the NIC:

```
telnet nic.sri.com
```

Follow the instructions to peruse the menus and other information that is available. Once you have found a file of interest, you can copy it from the NIC to your local computer by using the ftp (file transfer protocol) program:

```
ftp nic.sri.com
username: anonymous
password: guest
get filename
bye
```

The ftp program also has a help facility; just type help for a summary of the available commands.

INTERNET is the fastest growing of the United States networks and presently is supported by DARPA, the National Science Foundation, NASA, the Department of Energy, and the United States Geological Service. NSF has the mandate to support national networking for the scientific research community. The NSF communications backbone was upgraded in July 1988 with new gateways and high speed T1 lines (1.544 Mbits/sec). This backbone connects supercomputer sites in Princeton, Ithaca, Pittsburgh, Urbana, Boulder, and San Diego. In addition there are backbone nodes in Ann Arbor, College Park, Houston, Lincoln, Palo Alto, Salt Lake City, and Seattle.

The NSF backbone services the main node sites and a hierarchically structured set of mid-level networks: regional networks such as NYSERNET and NorthWestNet, consortia such as SDSC and JVNC, and affiliates such as BITNET and CSNET. Formal agreements between NSF and other agencies (DARPA, NASA, DOE) further facilitate communications. All of the mid-level networks support communications with at least 56 kbits/sec links.

The NSF supports network connections and the regional and consortia networks connect university campuses. Each campus is expected to provide local network connections and assistance to, any campus department that needs network access. This policy provides a level of local control yet supports connections at high speed. All of the campus links have 56 kbits/sec lines at minimum, and most campuses have one or more 10 Mbits/sec Ethernet Local Area Networks (LANs) on campus, making access quite simple.

Further information about INTERNET sites, services, and campus and regional coordination can be obtained from the NSF Network Service Center (nnsc@nnsc.nsf.net). Sites or facilities wishing to connect should send their postal address to the Program Office (dncri@note.nsf.gov). On-line information about NSF sponsored network services and facilities can be obtained from the NNSC. Mail a message to info-server@nnsc.nsf.net that contains the lines:

```
request: nsfnet
topic: help
```

Other topics (what-is-nsfnet, sites, coordinators, networks, etc.) are also available and may be requested on successive lines.

BITNET/EARN

BITNET (the name is derived from the phrase "Because It's Time") is a worldwide network connecting over 1000 hosts by means of released 9600 baud telephone lines. Funding used to be provided by IBM Corporation, but user sites must now foot the bill for their BITNET network traffic. IBM's RSCS (Remote Spooling and Communications Subsystem) protocols are used. The network has different names in different countries: BITNET in the USA (more than 1000 hosts in 1988), NETNORTH in Canada (91 hosts), EARN (European Academic Research Network) in Europe (363 hosts), and ASIANET in Japan (7 hosts), but these distinctions are invisible to the user. The network has a tree-like structure with the trunk at host CUNYVM in New York, and there is just one route between any two hosts.

Host names are non-hierarchical and are limited to 8 characters. Within EARN there are some conventions about how these names are constructed. For Austria, Germany, Sweden and Switzerland, the first character of the host name is the international country abbreviation (i.e., 'D' for Germany), the second and third letters are an abbreviation for the location, the fourth to sixth letters are the initials of the organization, the seventh letter is the number of the software version, and the

eighth letter is a system number (1 - 9, A - Z). Other European countries follow related conventions.

Consequently, most EARN names are unpronounceable and unmemorable, and there is often confusion between the letter 'O' and the digit '0'. For example, dgaeso51 is the host name for the European Southern Observatory, Garching, West Germany, hlerul51 is the Sterrewacht Leiden in The Netherlands, and ukacrl is the Rutherford Appleton Laboratory in England. Note that the Netherlands is denoted not by nl but by h (Holland).

Correspondents may refer to their host machine in a number of non-standard ways. For example, an EARN host at the Institutd'Astrophysique in Paris (friap51) might be referred to as friap51, or as earn.friap51, or as friap51.earn, or as iap51 on the FREARN network). Likewise, hlerul51 might be referred to as lerul51 on the HEARN network, and secthf51 as ecthf51 on SEARN. When sending BITNET mail you should use the standard site address, i.e., hlerul51 for Leiden.

The single EARN host in the United Kingdom, ukacrl, serves as a gateway to the JANET network. It relays mail only between JANET and proper BITNET hosts; it will not forward mail sent through another relay to BITNET. On BITNET in the United States the names tend to have more obvious meanings. For example, alaska is the University of Alaska, nrao is the National Radio Astronomy Observatory, and uwaphast is the University of Washington Physics Department. Sometimes BITNET hosts are referred to as host.bitnet. The .bitnet may usually be omitted in electronic mail addresses totally within the BITNET network. Because BITNET/EARN is IBM-based, characters sent from other types of machines may be translated from ASCII to EBCDIC, and "exotic" characters such as { _ # may be corrupted.

In February, 1989, the BITNET membership and CSNET board and trustees approved the merger of the two networks. A transition team is working to implement this decision. The merger will start with the administration of the two networks. It is not clear yet what all the implications of the merger will be.

For more information about BITNET contact info@bitnic.

SPAN

The NASA-supported Space Physics Analysis Network began operating in 1981. There are now more than 1000 hosts on the network, including 90 on the European SPAN segment. SPAN uses the DECnet protocols, and almost all of the machines in SPAN are DEC VAXes. The backbone of the network is provided by 4 routing centers connected by 56 kbits/sec links: NSSDCA at Goddard Space Flight Center in Greenbelt, Maryland, SSL at Marshall Space Flight Center in Huntsville, Alabama, JPLLSI at Jet Propulsion Laboratory in Pasadena, California, and JSC at Johnson Space Center in Houston, Texas. Most SPAN sites are connected with 9.6 kbits/sec lines.

The network is managed by the National Space Science Data Center (NSSDC) at GSFC. There is a transatlantic X.25 link between MSFC and the main host in Europe, ESOC (the European Space Operations Centre at Darmstadt). The Rutherford Appleton Laboratory is also a SPAN host (RLVAD). The names of hosts on SPAN may have up to 6 alphanumeric characters. For example, BKYAST is the Astronomy Department at U.C., Berkeley, CFAPS1 is the Planetary Science Division at the Center for Astrophysics in Cambridge, Massachusetts, EXOSAT is the EXOSAT project at ESTEC, The Netherlands, and GAL is at the NASA Ames Research Center.

Hosts also have numbers of the form area.machine, where area is a 6-bit area code. You may need to specify the SPAN address in its numeric form if your site does not have a current SPAN site table. One can determine the numeric form of a SPAN address from the formula 1024 x area + machine. For example, cfaps1 is SPAN host number 17.32, corresponding to address 17440 in decimal. JANET users should note that the number may not be used as a substitute for the name when sending messages through the gateway at star.stanford.edu, although most other gateways accept them. Addresses on SPAN (and other DECnet based networks) are given in the form host::user or, if routing through machine host1 is to be specified, as host1::host::user. Using the routing may be handy if your computer doesn't have the host name in its site table and you don't know the number or if you know a certain routing is better or if one of the normal links is down. Remember that mail cannot be delivered over SPAN unless the full link between you and the distant user is up and working. Note that SPAN is integrated with the HEPNET, the High Energy Physics Network (see Section 2.7). HEPNET addresses have the same form as SPAN addresses, i.e., host::site. For information about SPAN, loginto host nssdc, userid span_nic. For more information contact SPAN Project Manager, Code 633, NASA Goddard Space Flight Center, Greenbelt, Maryland 20771.

*(to be continued in next **CACHE News** issue)*

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.

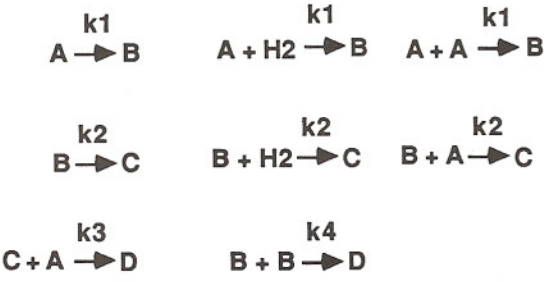
In order to edit the column efficiently, the submissions must be made to Finlayson via BITNET, address FINLAYSON@MAX or on a diskette in ASCII. He will acknowledge receipt of the submission via BITNET, and will send the edited column to the CACHE office via BITNET. Letters will not be accepted. This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

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:



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.

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

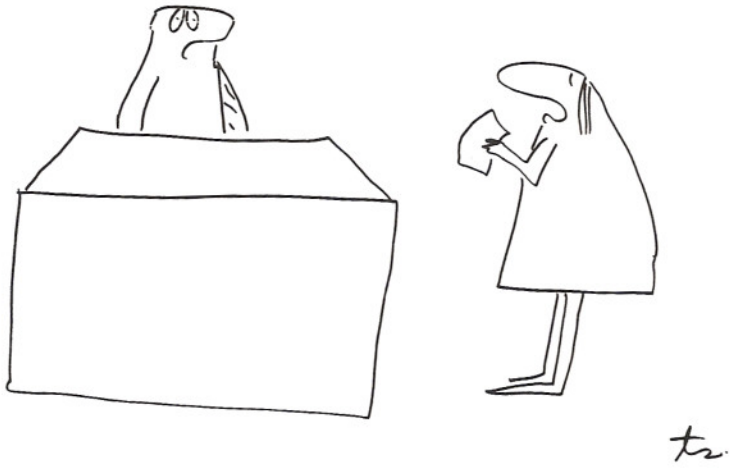
9. MIDAS - Microcomputer Integrated Distillation Sequences No. 26 and 27,
   Andrew Hrymak, McMaster University

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,
    by Alan Foss, University of California, Berkeley

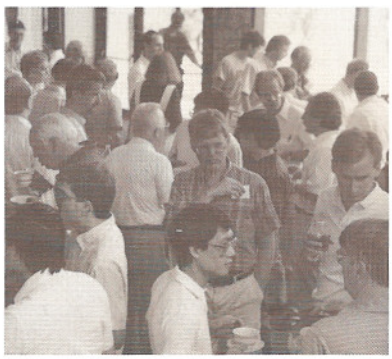
13. Real-time Dynamic Distillation Simulation and Relative Gain Program No. 27 and 28,
    by Alan Foss , University of California, Berkeley



"If a test installation functions perfectly, all subsequent systems will malfunction."

Focapd '89 Conference Report

The third Foundations of Computer-Aided Process Design conference was held in July in Snowmass Village, Colorado. The conference, cosponsored by CACHE, the CAST division of AIChE, and the National Science Foundation drew 170 academic, industrial, and governmental attendees from the United States and 18 foreign countries. For the first time, a number of graduate students were also invited to participate.



Discussion at Coffee Break

The technical sessions included design theory and methodology, artificial intelligence applications in process engineering, chemical process synthesis, nonlinear systems analysis, batch and retrofit design, process engineering environments, chemical and nonchemical product design, recent process design research results, and speculations on the future of the discipline. In addition, five process engineering software vendors demonstrated their products throughout the week.

Keynote Speaker Wozny

Continued discussion at break

In the tradition of the previous CACHE/CAST/NSF conferences, the lengthy question-and-answer periods, the ad hoc afternoon special sessions, and the intense hospitality room discussions (one lasting until after 4:30 a.m.) contributed to what was by all counts a very worthwhile meeting experience (or was it just the conference barbeque and the western hats?)

Stephanopoulos and daughter

ANNOUNCEMENTS

New FORTRAN Codes

W. E. Schiesser
Lehigh University

(1) DSS/2 , a transportable FORTRAN 77 code for the numerical integration of ordinary and one, two, and three-dimensional partial differential equations, is now available in the following machine-readable formats:

(1.1)Nine-track tape

(1.2)DOS-formatted, 5.25 inch, l.2 mb diskettes

(1.3)DOS-formatted, 3.5 inch, l.2 m diskette

In each case, FORTRAN source code, written as ASCII files, is provided. Details for the purchase of DSS/2 are available from: Dr. W. E. Schiesser, Mountaintop Campus, Building A (111), Room D307, Lehigh University, Beth-lehem, PA 18015 USA, (215)758-4264, E-mail: WEST@-LEHIGH.BITNET, FAX: (215)758-5423.

(2) A global CO_2 model, written in transportable FORTRAN 77, is available in either format (1.2) or (1.3). The model represents the exchange of CO_2 between seven well mixed reservoirs: the upper and lower atmosphere, the short and long lived biota, the mixed and deep sea layers of the ocean and the marine biosphere. The level of CO_2 in each of these reservoirs is computed as a function of time by the numerical integration of a system of initial-value ordinary differential equations. Factors affecting the CO_2 distribution in the atmosphere can be evaluated, such as increased fossil fuel burning and the destruction of forest areas. The model does not contain a climatic component, and cannot be used to study the radiational balance between the earth and space.

The model is available as FORTRAN source code, written as a series of ASCII files. The one-time, site license price is $100.00. Please enclose a check, payable to Lehigh University and mailed to W. E. Schiesser at the address indicated above.

Multicomponent Stage-to-Stage Distillation for Microcomputers

Paul Barton and Matthew K. Frazier

Distillation, Multicomponent, Stage-to-Stage is a user-friendly, interactive, distillation design package for IBM-compatible PCs with minimum 256K RAM. The program is written in BASIC.

The program rigorously solves material balance, heat balance, and equilibrium equations for multicomponent (up to 10), multistage (up to 100), continuous fractionation with single or multistage feeds. The equilibrium models are based on perfect gas, and ideal liquid solution or regular solution solubility parameter. The program calculates: number of stages; feed stage locations; product rates and compositions; stage temperatures and compositions. Column inputs are: compositions, temperatures, and phase states of the feeds; column pressure profile; reboiler heat; column heat-loss profile; Murphree stage efficiency; predesignated over-all separation desired for the key-pair constituents. Physical property inputs for each component are: coefficients for vapor-pressure equation; solubility parameter as function of temperature; vapor heat capability, liquid heat capacity, and latent heat of vaporization at two reference temperatures.

Initial guesses are required for product rates and compositions. The calculation routine is based on the stage-to-state bottom-to-top procedure. The material balance, heat balance, and equilibrium equations are solved iteratively on each stage, one-stage-at-a-time. Novel algorithms are used to promote convergence from one column pass to the next.

The degree of rigor is adequate for many commercial design situations. Ease of convergence makes this program useful for generating good input data for the more rigorous programs that are difficult to converge. This program is ideal for observing and teaching the basics of distillation column performance, especially in the "print every iteration" output mode.

A diskette with instruction manual may be purchased for $35, payable to Paul Barton. Send requests to Paul Barton, P.E., Box 158, RD 4, Bellefonte, PA.

The POLYMATH Numerical Computation Package

Mordechai Shacham

POLYMATH is a numerical computational package that Professor Cutlip of the University of Connecticut and I have developed. We have been using this package for about seven years as a computational tool in both graduate and undergraduate courses. The package is now being made available for all the Chemical Engineering Departments via CACHE.

The package consists of the following programs:

MATRIX MANIPULATOR evaluates matrix expressions containing all basic operations, solves linear equations, and determines eigenvalues/eigenvectors.

NONLINEAR EQUATION SOLVER handles up to twelve simultaneous linear and nonlinear algebraic equations.

DIFFERENTIAL EQUATIONS SIMULATOR solves up to twelve simultaneous first-order ordinary differential equations.

CURVE FITTING PROGRAM fits polynomials up to the 5th order and cubic splines directly to entered data of y versus x. User-provided functions can be invoked to transform the data before fitting.

MULTIPLE REGRESSION PROGRAM fits mathematical models containing up to five linear parameters to data consisting of one dependent and up to four independent variables.

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

The package runs on IBM PC/XT, AT, PS/2 and most compatibles. It requires a color graphics board: CGA, EGA, VGA or Hercules. In the Ben Gurion University, students are introduced to POLYMATH in one, hour long session. They are provided with the program disks and a three page handout describing the installation and execution of POLYMATH. During the one hour session the students install POLYMATH on their computer and solve one sample problem from each of the following categories: nonlinear algebraic equations, ordinary differential equations and polynomial curve fitting. As a homework assignment, they have to solve three additional problems from the three categories. After this introduction they continue to use POLYMATH in many of the courses they take, in the senior project, and even in their research project (graduate students), without any additional help.

We hope that the use of POLYMATH will be as beneficial to the faculty and students of the other ChE departments as it is for ours. We expect that the capability of solving realistic problems efficiently will have a major impact on chemical engineering education by shifting the emphasis from the technical details of the computer solution to the formulation/analysis of the particular problem. The computer disks should be available in 1990.

References

1. Shacham, M. and M. B. Cutlip, "A Simulation Package for the PLATO System," Computers and Chem. Eng., vol. 6, no. 3, pp. 209-218, 1982.

2. Shacham, M. and M. B. Cutlip, "Applications of a Microcomputer Computation Package in Chemical Engineering Education," Chemical Engineering Education, vol. 12, no. 1, p. 18, 1988.

3. Shacham, M., M. B. Cutlip, and P. D. Babcock, "A Microcomputer Simulation Package for Small Scale Systems," Microprocessors and Microsystems, vol. 9, no. 2, pp. 76-81, 1985.

Status of Flowtran Load Modules For University Computers

J. D. Seader

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

CACHE continues to supervise the preparation of FLOWTRAN load modules for some mainframe, supermini, and supermicro type digital computers and the distribution of the modules on magnetic tape to departments that order them. A new optimization feature is not included, and the instructional FLOWTRAN book is now in its third edition. Please see the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

DEC VAX computers running with the VMS and ULTRIX operating systems.

DEC 20XX mainframe computer running with the FORTRAN-20 compiler (9-track, 1600 BPI tape).

UNIVAC 1100 series computers running under the EXEC 1100 operating system with the FORTRAN compiler (9-track, 1600 BPI tape).

Amdahl computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).

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

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	OS1/MVS	IV-H ext.
c	OS/VS2 MVS	VS
d	CMS	IV-G1

IBM PC-XT 370 PC operating in conjunction with an IBM mainframe.

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

Apollo Domain work stations running with AEGIS operating system (program on floppy disk).

Data General MV superminicomputers running with the AOS/VS operating system.

Honeywell computers with CP6 operating system.

Sun work stations running UNIX Encore Multimax APC.

Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes but not for consulting. One hundred and fifty-six FLOWTRAN tapes and floppy disks have already been distributed.

If you would like to obtain a FLOWTRAN tape for your computer and have not already contacted CACHE, complete and submit the FLOWTRAN TAPE form on page 33. You will be required to sign a User's Agreement that must be approved by Monsanto. The cost of the tape, payable to CACHE, is $250. The charge to CACHE-supporting departments is $175.

FLOWTRAN BOOKS

Send to:
ULRICH'S BOOKSTORE
Attn: Heather Senior
549 E. University Avenue
Ann Arbor, MI 48109

Please send me:
NAME_____
Flowtran Simulation—An Introduction,
3rd edition; Pauls.
ADDRESS_____

_____

No. of copies_____ @ $16.95 copy

_____

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

FLOWTRAN TAPE

____**I am interested in preparing a FLOWTRAN tape.**
____**I am interested in obtaining a FLOWTRAN tape.**

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

_____

2. Operating system version:

_____

3. FORTRAN compiler version :

_____

4. Magnetic tape facility:

No. of tracks_____

Drive speed in bits/inch_____

Name: _____
Send form to:
Professor J. D. Seader/CACHE
3290 MEB
University of Utah
Salt Lake City, UT 84112
Send this form only if you have not previously contacted Professor Seader.

Eurecha Teaching Programs

The Eurecha Teaching Program Project collects and distributes chemical engineering programs to teaching institutions. The modifications make the programs suitable for almost all machines with FORTRAN compilers, and can be used interactively or in batch mode.

Programs available:

1.	CHEMCOSET:	Data bank
2.	UNICORN:	Flowsheet programs
3.	DISTILSET:	Distillation programs
4.	THERMDINSET:	Thermodynamics
5.	CAPCOS:	Capital cost estimation package
6.	TACS:	Simulation of control systems
7.	VLESET:	Comprehensive VLE analysis package
8.	DIAGNOSE:	Chemical plant fault diagnosis exercises
9.	SYSNSET:	Heat exchanger network and column sequencing
10.	STATCHAR:	Statistical charac terization of analytical results
11.	BATCHDIST:	Batch distillation design program
12.	INTERN:	The designs of column internals
13.	REACTEX:	Eleven reactor models suitable for running alone or as UNICORN subroutines. All have been used as the basis for student design projects.
14.	REACTPELL:	A heterogeneous solid/gas catalytic model of the partial oxidation of benzene to maleic anhydride.
15.	ENISYN:	Synthesis of energy integrated distillation systems.
16.	OPTIMISER:	Non-linear optimisation in chemical engineering
17.	REPROCHE:	Non-linear regression program.
18.	CHEQUUS:	Chemical equilibrium calculation.
19.	KINET:	A kinetic examination, data acquisition and regression program

For further information please write:

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Hochschule (E.T.H.), Swiss
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Chemisches Laboratorium
Chemical Engineering Dept.
CH-8092 Zurich
Switzerland

Call For Proposals for the Preparation of CACHE Process Design Case Studies

Over the course of the last four years the CACHE Process Design Case Study Task Force has published the following four case studies:

1. Separation System for Recovery of Ethylene and Light Products from a Naphtha Pyrolysis.
2. Design of an Ammonia Synthesis Plant.
3. Design of an Ethanol Dehydrogenation Plant.
4. Alternative Fermentation Processes for Ethanol Production.

These case studies are being used in many universities and have been well received. As a result, CACHE is seeking to expand the project to include high quality contributions from our faculty colleagues at large. In fact, a new case study is currently under preparation in response to our call for proposals in 1988.

We are seeking new proposals for the development of a CACHE Process Design Case Study and are willing to provide funds up to a maximum of $5,000. This money can be used, for example, to pay the stipend of an undergraduate/graduate student, to contribute to the summer salary of the supervisor or to cover other office expenses.

Proposals of interest include nontraditional chemical engineering tasks (e.g., semi-conductor processing, bio-processing and materials), batch processing, retrofit design and waste minimization. Projects with industrial participation are viewed favorably. Proposals should be directed to Professor Manfred Morari, Chemical Engineering 206-41, Caltech, Pasadena, CA 91125 and Professor Ignacio E. Grossman, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213.

As a reminder, the goal of the Design Case Study Task Force is the development of case studies to aid process design education. Though no two design problems are alike, there is a general logical sequence of basic steps which lead to a good design. It is the chief objective of the CACHE Case Studies to demonstrate and elucidate this thought and decision process. The CACHE Case Studies should be different from final student or industrial project reports in that they do not only present one final solution, but show the whole solution procedure leading form the problem statement to the final solution(s) in an organized manner. Within that philosophy, neither is the scope fixed nor the methodology limited. Eventually, a library of case studies is sought ranging from small ones to large ones and covering a variety of design aspects.

For more details, please contact Manfred Morari or Ignacio Grossman.

CACHE Process Design Case Studies

The new CACHE Case Study Vol IV: "Alternative Fermentation Processes for Ethanol Production" is now available. The objective of this case study is the design and evaluation of several different processes for ethanol production. The intent is to expose the students to some nontraditional chemical engineering processes and to introduce them to the rapidly expanding field of biotechnology. The project deals with the integration of a process flowsheet where a number of alternative fermentors are considered. A floppy disk is enclosed for the simulation of the fermentors as well as the input file for the process simulator FLOWTRAN. The case study was developed by Professors LeBlanc and Fournier at the University of Toledo.

In addition to the new case study, the first three volumes are still available for purchase. All case studies are $35 including postage (book rate in the U.S. and surface mail for orders shipped overseas). The initial copy for departments that support CACHE is $15.

(Please see ordering coupon on next page.)

Chemical Process Control IV (CPC IV)

Planning for CPC IV is forging steadily ahead. The proposed date is February 17-22, 1991 at South Padre Island, Texas. Harmon Ray and Yaman Arkun are the conference co-chairman, and Tom Edgar the CACHE coordinator. The conference will have exclusive use of meeting and dining facilities. Details of the program will be available in 1990.

Vol. I: Separation System for Recovery of Ethylene and Light Products from a Naptha Pyrolysis Gas Stream
No. of Copies:_____

Vol. II: Design of an Ammonia Synthesis Plant
No. of Copies:_____

Vol. III:Design of an Ethanol Dehydration Plant
No. of Copies:_____

Vol. IV: Alternative Fermentation Processes for Ethanol Production
No. of Copies:_____

Name_____

Address_____

_____

Please mail this form to:
CACHE Corp.
P.O. Box 7939
Austin, TX 78713-7939

Make checks (U.S. funds, U.S. bank) payable to: CACHE Corporation.