Computing and Systems Technology Division



Communications

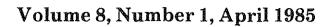


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About This Issue

In the April 1985 Communications, we feature three articles: the award address of Professor Rex Reklaitis (Purdue University) at the CAST Division banquet in San Francisco last November; a discussion, by Professor Rudy Motard (Washington University at St. Louis), of data base management in engineering; and a description, by Gerald Jacobs and Ernest Henley of COADE, of a new generation of user-friendly process simulators that are oriented toward personal computers.

The Editor and Arthur Westerberg (Carnegie-Mellon University) discuss the CACHE National Electronic Mail Experiment in the News section of this Issue. We solicit all CAST Division members to join us in these early stages of the development of a worldwide chemical engineering network that can be accessed by anybody in industry, academia, or government.

Sample items from the CACHE Newsletter Microcomputer/Personal Computer Notes are given in the News section as an experiment to determine if you are interested in such information; please let us know.

CAST Communications continues its recent tradition of experimentation (initiated by our previous editor, Dr. Edward Gordon of Fluor Engineers, Inc.) with a new title, a modified appearance, a new method of layout, an improvement in texture (inclusion photographs), the electronic transmission of keystrokes, AIChE as our new printer/mailer. What prompted these changes? The answer is the report, The Newsletter Format Option (parts of which are reproduced in the News section), written by Charlotte Guthrie (UCCEL Corporation) and presented by her to the CAST Executive Committee at the 1984 Anaheim AIChE meeting. In this Issue, we test her recommendations for the cover page, the segregation of section contents,

and the use of both three-column format and smaller-size type.

In addition to thanking Charlotte publicly for her important input into the CAST publications process, Ed Rosen, the CAST Division Chairman, and Peter Rony, Editor of CAST Communications, are pleased to announce that she will continue her participation on the CAST Publications Board as an Associate Editor for CAST Communications.

The layout of this Issue was performed by Joe Wright (Xerox Research Centre of Canada) and his secretary, Debbie MacPhail, who employed a Xerox 8010 Star Workstation for the final layout process. We used electronic data CAST transmission send to Communication disk files from the Editor's Zenith Z100 personal computer in Newark, Delaware to Joe's computer in Mississauga, Ontario.

The printing and mailing of this Issue was handled through AIChE headquarters, which has been routinely performing this task for the twelve divisions of AIChE. Cameraready copy, courtesy of Xerox Research Centre of Canada, was sent to Barbara Boyer (AIChE), who did the rest.

The CAST Publications Board thanks Timothy B. Challand, of Simulation Sciences, Inc., for his enthusiastic behalf of CAST work on Communications. We also thank our this Issue: Rex contributors to Rudy Reklaitis. Motard, Gerald Jacobs, Ernest Henley, Arthur Westerberg, and the Programming and Area Chairmen.

Our tentative deadline (which we did not meet) for the mailing of this Issue was the spring AIChE meeting, which was held very early this year (March 20-24 as compared with May 20-23 in 1984). The fall Communications will be mailed near the end of October; our absolute deadline for final copy is September 15, 1985. It will be a theme

issue on networks in academia and the Tentatively scheduled is an CPI. article based upon excerpts from, BITNET-Because It's Time, by Ira Fuchs, Vice Chancellor for University Systems at the City University of New York. We solicit your articles on networking at your companies, your questions about this subject, news CAST items. programming information, and so forth. If possible, please transmit all material for CAST Communications electronically directly to the Editor (P.RONY or **Editors** RONY) Associate or (C.GUTHRIE or J.WRIGHT) through the electronic mail service. COMPMAIL+, with which CACHE is experimenting. We can give you details about the special CAST account that we are creating for such a purpose.

CAST Chairman's Message: Planning, Planning

Long range planning has now become a routine activity of the CAST Executive Committee. At the San Francisco CAST meeting, the long range plan was accepted and will be implemented in 1985.

The plan has several elements which will ensure that CAST will continually address new issues and ideas. Each year the new First Vice Chairman will join the first year Directors and selected members of the CAST Executive Committee to re-think the The second-year long range plan. Directors will work on membership while the third-year Directors will address special issues such electronic bulletin boards and the speakers' bureau. The Second Vice-Chairman chairs the Awards Committee while the Chairman makes sure it all works.

In addition to the assignment of specific duties for the Directors, the plan addresses some of the major issues facing CAST. One of these issues is that of publications. The plan calls for making non-archival material available to the CAST membership—the material generally appearing in our current CAST Communications.

CAST Communications was the topic of considerable deliberation in San Francisco. Dr. Ed Gordon of Fluor. who has been the Publications Board Chairman responsible for Communications, reached the end of his appointment. Dr. Peter Rony of Virginia will fill Tech that appointment for 1985-86. The problem is one of publishing a rather substantial document without calling upon any one individual's major time commitment. In order to save costs, this has often been done utilizing corporate facilities various considerable volunteer time.

In order to relieve the Editor of some editorial responsibilities, an offer was considered from Pergamon Press (the publisher of Computers and Chemical Engineering) to publish CAST Communications. Because of considerable opposition, however, the offer was rejected.

The publication issue for non-archival material is not yet resolved. The archival area is in much better shape with Computers and Chemical Engineering and the plans to expand the AIChE Journal to a monthly publication in 1985. We shall hear more of this issue in the future.

In the meantime, we have another option in mind. Would you be interested in receiving each year a two-volume CAST Proceedings that contains reprints of papers presented at the spring and fall AIChE meetings? Please give us your reaction, pro or con, to this idea, which is discussed in further detail on the survey form at the end of this Issue of CAST Communications.

Edward Rosen, Chairman, CAST.

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Perspectives For Computer-Aided Batch Process Engineering

Professor G. V. Reklaitis, Purdue University, West Lafayette, IN 47907

Under these circumstances it is traditional to give a speech offering sage comments on the history of the technical progress in some field of and CAST application to issue profound forecasts of future developments and trends. A plaque and access to a podium apparently are supposed to give an individual the perspective and temerity he otherwise does not have to make such sweeping generalizations. I will, of course, uphold this tradition, although I should warn you that the superior powers of the CAST plaque seem not to have descended upon me-yet.

The area upon which I have chosen to focus attention is the application of computing technology to batch processing. In the brief time period allotted, I will try to convey to you three basic points:

- 1. Why is it that batch processes are of interest today?
- 2. What is it that has been accomplished to date in the way of computer-aided methodology for this category of processes?
- 3. What are some of the more interesting future possibilities involving the application of computer technology to batch process engineering?

First, why should we be interested in this form of chemical processing? What relevance does it have to the future? Without question, batch processing has dominated the history of chemical manufacture for hundreds of years. It is only for the last 25 years that it has been virtually banned from chemical engineering textbooks. What is remarkable to me is that this ancient form of processing is of

relevance in the high tech era for nearly the same reasons that led to its initial use centuries ago: (a) the desire to make money by producing materials which are viewed to be exotic by the customer and hence fetch a high price, and (b) the resulting need to produce fairly complex chemical products from a relatively poor engineering information base. Lets look at a historical example to help clarify these points.

"It is only for the last 25 years that it [batch processing] has been virtually banned from chemical engineering textbooks."

As you know, gunpowder was produced from saltpeter, charcoal, and sulfur by the Chinese as early as the tenth century. It was introduced in Europe as early as the thirteenth century, but there was one big supply problem faced by most of the European producers. namely, the absence of adequate natural deposits of saltpeter, or To solve this potassium nitrate. problem a batch process was invented by some unknown proto-chemical engineer. The key element of this process was a batch reactor called the niter bed. I should add that most of the European kingdoms required their land owners to set up such reactors, as did the Colony of Massachusetts of its plantation owners. The niter bed consisted of alternating layers of decaying animal and vegetable matter, mortar from old walls, earth and sand, all piled to a thickness of three to four feet on floors of wood or clay. The whole bed was covered to avoid rainwater leaching. periodically wetted with blood urine. The frequency and amount of this moistening were proprietary secrets, as no doubt were the precise origins of the moistening agents as well as the style of application. After two years of such fed-batch processing,

the batch reactions were considered to have been completed and the results ready for further processing. This leaching involved with containing potash, evaporation of the resulting solution, and repeated recrystallization. The typical yield from this batch process was about 0.3 lb of saltpeter per cubic foot of bed This level of every two years. productivity must also be fairly typical of present day pharmaceuticals processing, judging from the prices charged for some pills on the market. What is more remarkable is that this type of processing was carried out routinely for some 500 years basically by simple peasants with minimal supervision. This is probably where the batch industry got its tradition of using highly skilled operating labor and its inclination to plan for long production campaigns. It was done without the vaguest notions of the chemical kinetics and transport processes, or even of the chemical species or the stoichiometry which were involved. This tradition, too, seems to have been well preserved in certain sectors of the batch industry.

"Batch operation allows a reasonably safe scale-up from bench conditions without an extensive engineering knowledge base, by largely following laboratory recipes."

The actual processes taking place were of a biochemical nature: the bacterial conversion to nitrates of the nitrogen combined as urea or resulting from the decomposition of the animal or vegetable protein. On leaching with a solution containing potash (potassium carbonate), the nitrates were of course further converted to potassium nitrates. One really must wonder how the process ever was invented. What curious sequence of events led to the selection of the ingredients, the conditions, and the bed structure? Then, as now, serendipity clearly was crucial to process research.

"Batch processing offers a microcosm of computing applications that is as broad, if not broader, as the range of applications that arises in continuous processing."

I claim that conditions may not be all that different in the present day use of batch processing steps to make complex pharmaceuticals, specialty chemicals, and genetic engineering products. Batch operation allows a reasonably safe scale-up from bench conditions without an extensive engineering knowledge base, by largely following laboratory recipes. If need be, it is possible to operate with knowledge minimal of detailed properties, correlations, or semiempirical models. Furthermore, batch operations are risk isolating by nature-if a step fails to execute properly, only that batch is lost. Therefore, for nearly the same reasons that led to its invention in antiquity. plus reasons of economics and technical flexibility, batch processing is becoming the processing mode of the future.

Since the processing industries that employ this mode of operation are increasingly becoming subject competition-really a on basis-there does exist a genuine need for the development and application of computer-aided methodologies batch operations. This state of affairs has, of course, been realized by a number ofdistinguished researchers-notably Professor Rippin and Professor Hashimoto. Some interesting work has resulted from the independent efforts of these and other researchers, some of which I would next like to highlight for you. We are at the second point of the talk: the

state-of-the-art of computer aids for batch processing.

Batch processing offers a microcosm of computing applications that is as broad, if not broader, as the range of applications that arises in continuous processing. The areas include: the design of units and entire plants, the scheduling of processes, process control, and process management. Efforts in design optimization range from the cycle time optimization of single product trains to the sizing of multi-product plants. This has typically been accomplished using standard nonlinear optimization or branch-and-bound methods. Probably the most innovative work has been that of Sparrow, who formulated a good design heuristic for purely batch plants; the work of Mauderli, who presented an approach to multipurpose plant design; and the work of Hasebe, who studied the incorporation of intermediate storage design as part of the equipment sizing. The recent work of Yeh in devising new heuristics for the multi-product plant is also noteworthy. A rather comprehensive analysis of intermediate storage and its various roles, leading to results suitable for design, has been developed by Karimi; some of that work was reported today. The Batchmaster system, also described today by Mr. Preston, seems to offer a well thought out user framework for many of these calculations, and hence must be recognized as an important new development.

Much of the earlier work in process scheduling was notable for its lack of practicality. For example, with Chuck Forester we once were solving three parallel processor scheduling problems with changeover crew constraints and 20 products using integer programs which required thousands of seconds per optimization on a CDC 6500. While enumerative or branch-and-bound approaches still are discussed, much of the recent focus has been on the development of approximate

suboptimal methods such as those that will be reported by Wiede and others in Thursday's session. However, the repertoire of general algorithms available as yet is quite limited, involving simplified or specialized configurations. no resource restrictions, and performance-based objective functions. The most important lesson we have learned to date is that rigorous optimization of schedules is not a worthwhile goal.

"Much of the earlier work in process scheduling was notable for its lack of practicality."

The use of simulation to support design and scheduling activities is well established in the batch area. considerable literature exists on models for various batch unit operations. for example, batch distillation. However, this work typically does not extend to encompass process simulations. A number of studies have been published employing application-specific simulations using existing, especially discrete event, simulation languages such as GASP, or GPSS, or Simscript. For instance, the work reported by Felder this afternoon is of this type. The most interesting developments in this sphere are the design of flowsheeting systems for this class of processes: the UNIBATCH and BOSS developments reported earlier today. This work clearly has advanced beyond the proof-of-concept stage, but several more years of work remain to be done before these developments achieve commercial status.

In the control arena, a considerable literature exists on trajectory control of various batch operations; moreover, the application of batch sequencing controllers appears technically well established although not widely implemented. Interesting and important work remains to be done in

the computer control of complex batch operations such as fermentation, but this is application-specific rather than generic in nature. Process-wide control or the hierarchical linkage of the control and scheduling functions remains largely at the discussion stage. True computer-aided process management systems, complete with supporting automated process information data bases, have only begun to be discussed.

From this very cursory overview, it should be evident that the methodology has a long way to go before even the basic problems facing this sector of the processing industry will have been well solved. However, the gradient is distinctly upward and the prospects for major success are excellent! This brings us to the third and final point of this talk: a look at the future.

Where should we be directing our research efforts in the future? What major technologies should we be enlisting in order to accomplish our aim of computerizing batch process engineering?

In the design area the key topics of interest are aids for process synthesis, conditions especially under uncertainty. We need to take into account the important considerations that lead to the assignment of a sequence of processing subtasks to a given equipment vessel, to take into account the factors dictating the choice of location of intermediate storage in the processing network. We do need to take a concerted look at the plant-the multipurpose batch processing equivalent of a flexible manufacturing facility. Batch processing is used because of the flexibility it provides in accommodating to changing product state and product demand. We need to quantify that flexibility-to develop design procedures that synthesize networks and size equipment, taking into account uncertainty. The questions raised by Ignacio Grossman and Manfred Morari in the continuous processing environment certainly need to be addressed in the context of batch processing—although the required methods and formulations are likely to be quite different. The variability analysis for intermediate storage that Karimi reported today is an important, but still only a first, step in that direction.

"In the control arena, a considerable literature exists on trajectory control of various batch operations; moreover, the application of batch sequencing controllers appears technically well established."

In the simulation area we need to develop the logic that will permit greater flexibility to realistically represent real operations and their constraints. We need to provide capability for data-driven assembly of application-specific unit modules, both in terms of the description of the processing steps and the sequencing and event logic associated with these Of major concern is the enormous amount of data required to initialize and to run a realistic simulation case. In the case of the BOSS application discussed this afternoon, we heard of some 25,000 data entries required to define the simulation. Clearly, effective means must be devised for interactive menudriven input assembly, including linkage to separately maintained product recipe files, physical plant parameter files, and process initial condition information. Work is in progress in our group and elsewhere on these topics, but to my knowledge only at the level of pilot efforts.

Of perhaps even greater concern is the enormous amount of information generated by such a simulation-again the BOSS application involved some million data entries, which represented a one-week simulation history. The issues here are multiple: (1) Convincing someone who views the data that the simulation adequately represents the system. (2) Extracting useful information from such a large history file. (3) Understanding the trends that the simulation history data contain. (4) Comparing trends observed across a suite of cases.

"In the simulation area we need to develop the logic that will permit greater flexibility to realistically represent real operations and their constraints."

Many of these issues have been raised the steady-state flowsheeting context and the pat answers are data base management systems and computer graphics. However, the time-series nature of the simulation history information introduces some challenges not present in flowsheeting applications of DBMS methodology. user's need to readily and The interchangeably see plant-scale dynamics, individual operation dynamics, and resource utilization dynamics (raw materials, operators, utilities) present some interesting challenges for graphics software design. The simulation visualization and animation work carried out by Jon Maimon in our group, and by others such as ICI, appear to be very effective ways of enlisting the aid of interactive computer graphics. In this context, animation refers to the dynamically updated display of the changes of equipment status and transfers material quantities that occur batches proceed through the equipment network over simulated time. Animation helps in validating simulations: one can see whether the movement of batches through the network and the selection of units conforms to accepted plant practice. It also helps in understanding the results of the simulation, in identifying bottlenecks, and in spotting operator and other resource misallocations. Over the period of 3 to 5 years, developments in these simulation support areas will make the use of batch process simulation a routine matter for both design studies and. especially, for short term planning and debottlenecking studies in operating plants. With such support interfaces, plant simulations will become highly effective means of training operators. plant-floor supervisory personnel, and believe it or not, even managers.

"In the design area the key topics of interest are aids for process synthesis, especially under conditions of uncertainty."

In the area of scheduling and planning there is important research to be conducted that is of an algorithmic nature: develop methods for finding good schedules quickly-hopefully with some average or worst-case performance guarantees. The general network configuration, with various storage modes, product precedence constraints. and equipment restrictions. will require major continued research effort. Work is in progress in our group on a form of this problem and will be reported at PSE 85 next spring. But that really is only the beginning. The linkage of scheduling and materials-requirements planning needs careful consideration, since in batch processing the monitoring and preparation of ingredients is not merely an inventory function but actually is part of the normal plant floor activities of operators.

A major but very mundane need is that of automating the collection and assembly of plant status information. Clearly, without reliable plant information systems, scheduling

becomes an exercise in wishful thinking. With such systems it may actually be possible for management and staff to understand what is happening on the process floor. What a novelty that would be! Certainly. lot-tracking systems have been implemented in discrete parts manufacturing systems and sampletracking systems are in use in quality control and analytical laboratory applications. The transfer commercial scale batch operations will require creativity and inventiveness. but these are surmountable technical especially problems, with availability of shop-floor-hardened PCs and network capabilities. should see growing implementation of such systems over the next five years. Given the existence of such a system. an obvious possibility is to directly link the plant simulation to the process information base. Thus, the information base would automatically establish the initial conditions for plant simulations. With such a link, simulations could be routinely used to forecast potential operating difficulties or bottlenecks likely to be encountered before each period of operation is initiated.

"In the area of scheduling and planning there is important research to be conducted that is of an algorithmic nature: develop methods for finding good schedules quickly..."

In the area of process control, or more appropriately, computerized process operation, it seems that the most exciting development will be the integration of process information systems, the distributed unit sequencing and regulatory control functions, and the process scheduling methodology that we discussed earlier. This type of integrated process management technology is much

discussed in the continuous processing sector, and maybe even occasionally implemented. Unquestionably, this type of integrated process automation is highly appropriate in the multiproduct batch processing environment, with its high labor requirements and generally complex processing sequences.

"In the area of ... computerized process operation, it seems that the most exciting development will be the integration of process information systems, the distributed unit sequencing and regulatory control functions, and the process scheduling methodology ..."

This is not at all an outlandish proposal. Robots are being used today to perform the routine analysis task associated with quality control functions. The Zymark Corporation currently has some 200 small robots installed in industrial laboratory settings. These are basically singlearm devices that can pick up and move test tubes, operate syringes, and insert probes. Furthermore, as reported in the recent Industrial Symposium on Laboratory Robots, efforts underway to expand the role of robots in carrying out routine sample preparation. analysis, test tube cleaning, reagent injection. and reaction monitoring chores in a broader range of applications, such as organic synthesis. One such project is in progress in the Purdue University chemistry department. interesting feature of that work is the integrated use of the robot with microprocessor control to carry out an automated sequence of vieldoptimizing experiments. The robot can be programmed to automatically investigate a series of reagents and reagent concentrations using essentially a Simplex-type search strategy to guide its choices.

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A further interesting possibility is the automation of many of the manual functions arising in batch process operation through the use of robots.

Now it really does not take much imagination to envision robots performing operator tasks such as: (1) Extracting samples and initiating the analysis of these samples. (2) Cleaning out vessels between operations. (3) Coupling transfer lines to units. (4) Carrying out materials additions. (5) Disconnecting and moving product fraction collection vessels.

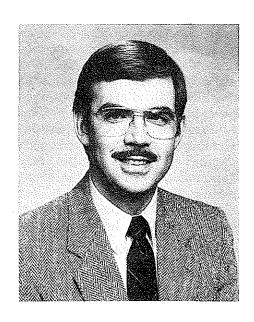
The use of robotics could reduce concerns with the exposure operating personnel to hazardous environments, could increase batch uniformity, and in the long run would substantially reduce operating costs. Of course, to realize this potential it would be essential that the operation of process robots be fully integrated with the unit sequencing and control functions. The result really would be the automated batch chemical plant of the future. Can you envision the irony? Good old batch processing would achieve a high tech status that would even be recognized by Time magazine! Unquestionably, this is a realistic and attainable goal since the robotics technology itself already exists.

In general, none of the research projects that I have discussed are technically or economically limited by hardware capabilities. The hardware required either exists or soon will be available. As pointed out recently by Ralph Gomory of IBM, computing power, memory, and display capabilities of computers can safely be projected to grow by 20% annually over the next five years. Clearly, in this case time is on our side. However, we, the members of CAST, will have to play the major role in achieving these levels of computerization because the major tasks are development of application-specific algorithms and systems. We should not expect parties

outside our field to understand our applications and to supply us with off-the-shelf hardware and software solutions. We just have to dig in and allocate the time and money to get the job done!

"A further interesting possibility is the automation of many of the manual functions arising in batch process operation through the use of robots."

In summary, I have tried to convey to you why in my personal view batch processing is an interesting and important area for computing-oriented research. We have taken a very brief look at what has been accomplished to date, and we have pointed to some directions for future research. I hope that I have conveyed to you the surprising breadth of topics that work in such an area encompasses, and thus hope that I have stimulated you to investigate further this growing area of application of computing and systems technology.



G. V. (Rex) Reklaitis, Professor of Chemical Engineering at Purdue University, gave the preceeding address as the recipient of the 1984 AICHE Computing in Chemical Engineering Award. He received his B.Sc. degree from Illinois Institute of Technology and Ph.D. degree from Stanford University. He is the author of two books, Introduction to Material and Energy Balances (1983) and Engineering Optimization (1983); an editor or co-editor of three ACS or AICHE Symposium Series volumes; and an author or co-author of 65 research publications. Most recently his research has focused on computer aids for batch/semi-continuous process design and analysis, and on applications of computer graphics. He is currently the Vice-President of CACHE Corporation.

Data Base Management For Process Engineers

Professor R. L. Motard, Washington University, St. Louis, MO 63130

Our profession has now experienced a generation of innovation in automatic computation, yet the field has never been as dynamic as it is today. New and powerful small machines, and the ability to connect workstations to each other and to large computers, have opened up new concepts of computer support for chemical engineers. Perhaps the most difficult choice that we face in exploiting these new trends is how to select the best products from a variety of commercial offerings. The other side of the problem, of course, is how to migrate from older generations computer systems. hardware. operating systems, and engineering computer programs to the newer environment. The new technology appears to offer so much more for potential interactivity, responsiveness, and integration.

Integrated Engineering Computing

By integration, I mean the ability to link together computer programs that work on different aspects of our database, much as a personal

today allows computer us to manipulate information in diverse ways at the touch of a button. We can enter data for display in a spreadsheet. analyze the consequences of "what if?" queries, prepare graphic images of the same data in different forms, move the data to a text processing program for a report, and store the information in a database management system, where it is ready to be extracted again by logical association. Many of us have marvelled at the facility of personal computers in dealing with these many representations of the same data: spreadsheet, text. graph, database. Naturally, we speculate what a similar integration could contribute to our work in process engineering.

Consider the following scenario. You have just completed a large process simulation model that contains a fractionator among many operations in the plant. You are not happy with the performance of the fractionator, and since the initial design parameters (number of trays, reflux ratio) were set by an educated guess, you decide to extract the fractionator model and its feed stream. You wish to suboptimize the trade-off between the number of trays and the reflux ratio. During the course of the case study, you must call in a sizing and costing program for the tower and its auxiliaries: condenser, reboiler, and reflux pump. You generate a graph of annualized cost (capital and operating) versus reflux ratio to make the final decision. All of this is done at workstation with simple commands. and the results returned to the database.

Later, a mechanical engineer completes the column vessel design and generates a vessel specification drawing to be issued for vendor quotation. In the meantime, a civil engineer has designed the structural steel framework for the fractionator unit and the concrete pad on which it sits. A plant design engineer becomes

engaged in developing a 3-D electronic model of the plant, placing the column, auxiliaries, valves and piping into a geometric database of the plant. In the meantime, drawings, documentation and reports to project management have been extracted and reviewed. All of this has taken place without ever moving data outside of the computer system.

What is the logical model on which information such an system developed? What do the gurus of personal computer software know that we can apply to the data being generated in process design and analysis? It is simply that data must be organized by information content and context and retrieved by the same logical rules. Data are to be saved and manipulated, not merely dumped onto computer printouts no matter how attractive the format. They are no that files pass through computer programs. Data provide a store of information against which one various plays transformations (programs) to elicit more information. down to the finest process detail.

We are engaged in research to adapt relational database management technology to the support engineering computing activities. will not go into more details on what a relational database system is; let us just say that it is one of the most efficient ways of organizing data and the information at service engineers. What I do wish emphasize are some ideas which form the basis for the power and flexibility of the coming generation of computer aided engineering and design systems.

Evaluation

From its earliest beginnings, engineering computation has been concerned with building modular software (in FORTRAN) that managed the flow of data through a sequence of computational steps chosen at the user's convenience. Flowsheeting systems are good examples. Later,

when some degree of integration was desired among several large software packages, workfile structures were developed which allowed any program to extract what information was needed, for its part of the overall task, from a common file of project data. There were some problems with this approach even though it was a simple concept. Whenever new data elements were added to the project workfile or whenever it was deemed necessary to change the organization of the data, many programs had to be revised since new access formats were required.

It then dawned on some engineers, who were aided by eager computer scientists, that database management techniques were needed to separate the data management function more cleanly from the computational function. The benefit was simply that the organization and complexity of the data reservoir could be altered and expanded without having to revise the computational programs. So far, so good, but now the programmers had created a system which still needed continuous maintenance; adding new data elements and organizations required that the data retrieval programs be revised even though the engineering programs were immune. Job security for the MIS people!

New data management concepts evolved, and today the buzzword is relational database management. which removes some of the problems encountered with the first-generation hierarchical and network (CODASYL) systems. Unfortunately, marketing hype has taken over a partially developed technology, and we are inundated with relational systems. It seems that there is nothing left to do but to select among a few available systems which claim to support engineering activities, and get on with our business. Nothing could be further from the truth! Most of the toy products on the market cannot be adapted the to management of engineering design, as many early attempts at integrated CAD have discovered to their chagrin. There is much yet to do.

Consortium Concerns

Embedded in the effort to separate the data from the programs are three aspects of engineering computing that must be accommodated. I refer to (1) computing per se. (2) the management of data, and (3) the logical structure of data as information or intelligence (the data model). Until we can assign a proper role to each of these three requirements we will not solve the problem of integrated engineering computing. These concerns form the basis for our industry/university Consortium on Engineering Design Management Washington at University.

We are engaged, with the financial assistance of several companies and the National Science Foundation, in a research program that seeks to adapt modern computer science to the needs in engineering the process industries. The Consortium produces prototype software for relational database management, data models in process and project engineering, and facilities for integrating existing programs into a total CAE/CAD environment: computing. data modeling, and management. The objectives are not to provide new engineering design programs, but to allow all existing software and CAD workstations to communicate with one another via a common data base using a set of generic data models.

There have been some attempts at databased engineering computing and, indeed, one can successfully link flowsheeting packages with equipment design software. Engineers are looking for a system which supports various kinds of consistency and constraint checking in the database. Graphical data must be coordinated with the information content of drawings. Different versions of the project data

be model (case studies) must maintained. Changes. updates. precedence of actions. and consequences of design decisions must be controllable. Imposing and checking of design rules and specifications must be facilitated.

Engineers are not the only persons accessing the database. One must provide consistent views of data when they are aggregated in different ways for managers, clerks, accountants, and schedulers. Many of the data objects in the database contain more than a few items. It may be necessary to collect hundreds of data items into a complex logical unit in order to make sense of something that one wishes to analyze to any degree of detail.

It is an ambitious objective, and I look forward to communicating more about our progress in the future.

The Application of Spreadsheets and Graphics to Process Simulators

Gerald Jacobs and Ernest Henley, COADE, A Division of International, Thomson Information Inc., 8550 Katy Freeway, Houston, TX 77024

A recent Wall Street Journal survey of businessmen who had purchased microcomputers showed a user product satisfaction of over 70 percent, the highest ever recorded for a hightechnology product. Until relatively recently, very few of the features that made microcomputers so popular so quickly in the business community-windows, help functions, menus, spreadsheets, and graphics-had been incorporated into engineering software for microcomputers. In general, the firstgeneration programs downloaded, mainframe programs that did not utilize the unique capabilities of the micros. Times are rapidly changing; the new generation of microcomputer software for engineers is starting to rival Symphony and Lotus 1-2-3 in visual and artistic display capabilities. As reported in another section of this Issue, a COADE presentation at the Houston meeting will feature 3-D stereoptic art.

An important practical implication of these technical advances is that computer programs, be they batch or interactive, are no longer command-language oriented. The casual user does not have to learn and retain a new language or consult a computer professional to use a program, and thus no longer has a major barrier to the enhanced engineering productivity

inherent in widespread computing usage.

Spreadsheets, menus, graphics, and pointing devices must, of course, be customized to specific engineering applications. In this brief paper, we describe some of the customization that was done to apply these techniques to a modern process simulation package, MicroCHESS, and a large pipe stress package, CAESAR II, both of which allow fullediting, user-activated screen mathematical functions. protection, cell intelligence, on-screen help windows, and elaborate graphic and spreadsheet inputs and outputs.

Menus

Menus are utilized for displaying multiple user options. They are driven by a pointing device such as a mouse or cursor location keys, which minimizes the errors inherent in having the user type in a number or letter. Two examples are shown in Figures 1 and 2. Note that the user-chosen option is highlighted, thus further reducing the possibility of errors to almost zero. In Figure 1, the shell or top-level menu is used to select the appropriate program phase, and in Figure 2 the phase of the flowsheet description is selected.

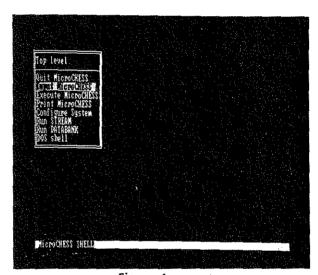
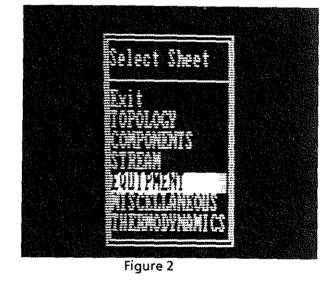


Figure 1



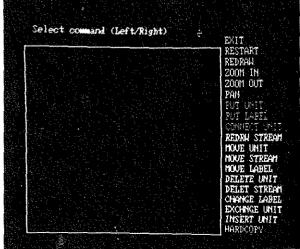


Figure 3

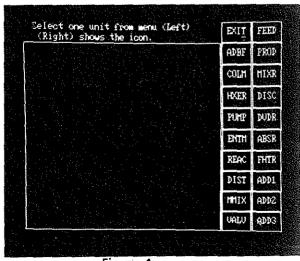


Figure 4

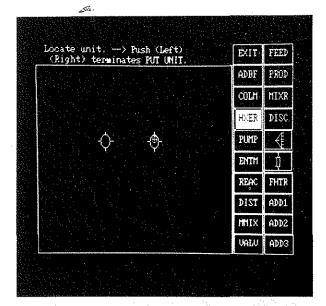


Figure 5

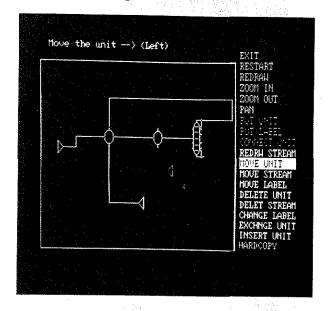


Figure 7

Graphics With desktop computing, connect time is not an issue so interactiveness can be fully exploited. Graphics can be used for process description, viewing of

results, data plotting, and report

generation.

Figure 3 shows the menu and "sketch pad" that the MicroCHESS user sees. If he says he wishes to create a flowsheet, he is shown the menu in Figure 4 and the graphical input phase begins.

Significant man-hour savings can be realized by freeing the engineer of the tedious job of sketching a flowsheet.

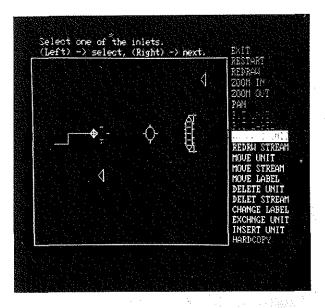


Figure 6

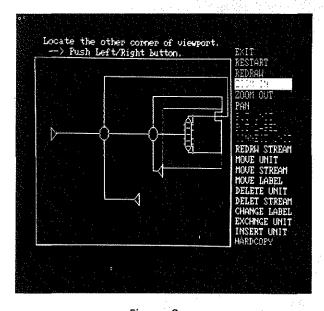


Figure 8

To create the graphical input, the user selects the appropriate unit and then, using the mouse pointer, he locates the appropriate symbol on the screen, as in Figure 5. Next the units are connected, again using the mouse (Figure 6).

After the flowsheet or technical factors are finished, esthetics or errors may necessitate the relocation of units. This process is shown in Figure 7. An important feature is the Zoom-in or Zoom-out function demonstrated in Figure 8 that allows the user to work on flowsheets of any size. For example, a flowsheet can be reduced on the

screen, and the printed output enlarged.

The user has the option of labeling streams and units (Figure 9) and of doing such things as moving units while maintaining stream connections, as shown in Figure 10.

The finished flowsheet is more than a "dumb" drawing. It serves as the input to the simulator whenever which the user defines stream and equipment parameters. All of the information on the flowsheet is automatically transmitted to the spreadsheet input. In addition, calculated stream data

and equipment sizing information can be overlayed on the flowsheet.

Spreadsheets

Process simulators require as inputs: (1) Process topology (connectivity); (2)

Stream information (temperatures, pressures, feed streams, chemical species); and (3) Equipment parameters (heat transfer coefficients, number of trays in a column). In MicroCHESS these inputs are

organized in a spreadsheet fashion, with on-screen help windows to guide the user in choosing the correct equipment parameters. Details are illustrated in Figures 11 and 12.

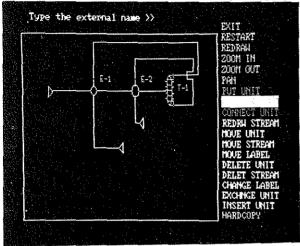


Figure 9.

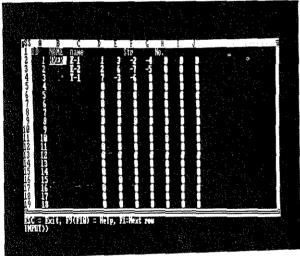


Figure 11

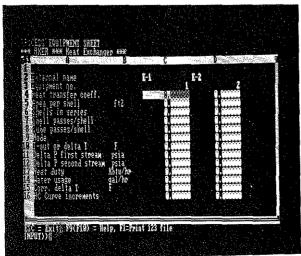


Figure 13

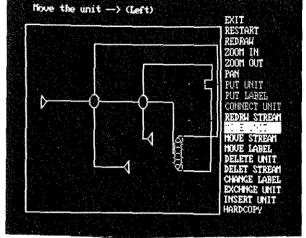


Figure 10

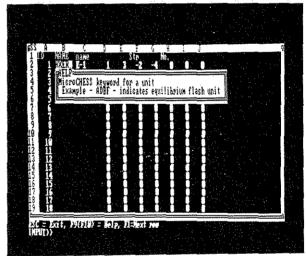


Figure 12

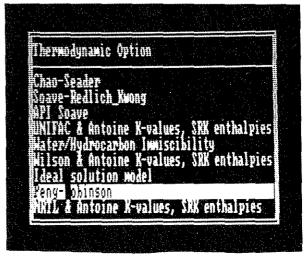


Figure 14

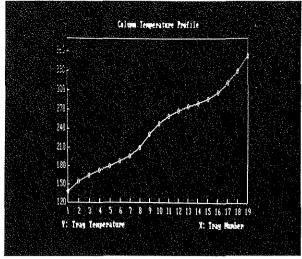


Figure 15

The spreadsheet input and graphic output both show process topology and interact in the sense that information on the flowsheet is automatically transferred to the spreadsheet. Conversely, the flowsheet can be automatically created from the spreadsheet. Partial transfer information is also possible. One can, for example, first draw the flowsheet without labeling streams or units, and then call the spreadsheet and number the streams. These streams and unit numbers will automatically the flowsheet transferred to internal program logic, that is, the user does not do anything.

Equipment parameters, as is the case for stream information, are in spreadsheet format. Note the use of guides (Figure 13) and menus (Figure 14), such as the thermodynamic options. Input errors are minimized by pointer selections, selected-variable flashing, and color coding.

Combined Graphics and Spreadsheets

The program output is, of course, the control focus of the engineer's interest. Combined graphic and spreadsheet output capabilities allow the user to study trends, manipulate data, transfer data, correlate variables, and make consistency checks. Figure 15 is a plot of tower temperature profiles created from tabular output. In Figure 16 we see a section of a piping network

1

in which the outputs are given the form of a graphical display along with tabular results.

The past two years have seen engineering microcomputer programs evolve from mainframe look-alikes to sophisticated communication tools that offer, in addition to computational educational and artistic power, interfaces that embody artificial intelligence and make full use of the unique features that contribute to the popularity amazing of microcomputers.

The CACHE National Electronic Mail Experiment

Peter R. Rony, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061

Arthur Westerberg, Department of Chemical Engineering, Carnegie-Mellon University, Pittsburgh, PA 15213

While selected chemical engineering professionals already have access to a computer network-most likely within a company but perhaps even a national network such as ARPANET or is BITNET-there currently national chemical engineering network between educational. industrial, and government institutions that is analogous, for

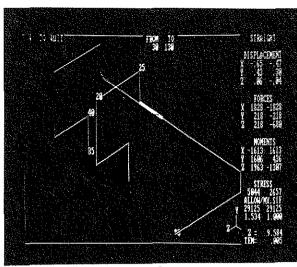


Figure 16

example, to CSNET, which is used by computer science and engineering professionals, or to COMPMAIL+, which is used by members of the IEEE Computer Society.

The objectives of the CACHE National Electronic Mail experiment are: (1) To catalyze the creation of a widely used national chemical engineering electronic mail network between academic, industrial, and government sites. (2) To extend such a network to our international colleagues. (3) To publicize the use of electronic mail in CACHE, CAST, AICHE, and other chemical engineering organizations. (4) To identify important uses for electronic mail in chemical engineering. (5) To perform limited tests of alternative electronic mail services. (6) To issue a report that documents examples of how to use electronic mail, identifies potential chemical engineering applications, and lists typical costs.

The COMPMAIL+ electronic mail service that we shall test is provided by ITT Dialcom, which serves 60,000 including Westinghouse users Corporation; Peat, Marwick, Mitchell and Company; American Bar Association: The White House: United States Department of Agriculture, Environmental Protection Agency, Food and Drug Administration, and Department of Energy; and IEEE Computer Society. The White House also uses ITT Dialcom's electronic mail

network for communications between the Office of Cabinet Affairs and more than 22 federal departments and agencies.

ITT Dialcom, with 800,000 messages per month and a 27% market share, is the second largest inter-company electronic mail vendor in the United States (Easylink, with a 33% market share, does not focus exclusively, as does ITT Dialcom, on professionals).

COMPMAIL+ has been selected for the CACHE National Electronic Mail experiment for several reasons:

- It can be accessed by anyone who has a terminal or personal computer and a 300-or 1200-baud modem. Access is not limited—as in the case of ARPANET, CSNET, or BITNET—to sites that possess network nodes.
- The costs are as low as \$6 per hour during non-prime time and \$16 per hour during prime time (1985 rates).
- A single site or entire organization can charge costs to a single group account (which can contain many individual accounts) that has a minimum billing of \$25 monthly.
- The minimum charge for an unused individual account (that is a part of a group account) is only forty cents per month.
- The COMPMAIL+ commands are simple to use. Only a subset-MAIL, SCAN, READ, SEND, FORWARD, REPLY, DELETE, QUIT, and OFF-is needed for most situations.
- Access is through TYMNET (preferred because of better quality message transmission), TELENET, UNINET, in Canada, DATAPAC and in the United Kingdom, IPSS.
- 300/1200 baud dial-up capability, with both ASCII and X.25 protocols and international packet switching service.
- Serves over 500 cities in the U.S. and over 150 cities abroad.

- Provides security through: (a) user ID mailbox with password, (b) user password control, (c) individual message password, (d) user ID security levels, (e) encryption using 6-letter key, and (f) file and program protection.
- Provides services such as: MAIL (electronic mail), WPMAIL (word processor mail), XMAIL (electronic mail/TELEX link), POST (electronic bulletin board, both public and private), CHAT (interactive electronic conversation), PARTICIPATE (teleconferencing system), and NET TALK (conferences involving up to 128 users at once).

These COMPMAIL + services provide:

- a. Mail drop capability, in which a user can send messages by a local phone call to a central computer in Maryland, which routes the message to the mailboxes of other recipients.
- b. Mailing list capability, in which a user can send his message to many recipients simultaneously, thus saving time and money. Electronic carbon copy capability also is provided.
- c. Quick response: a completed message is immediately placed in the mailbox of a recipient.
- d. **Message storage**: the ability to store both transmitted and received messages for later recall.
- e. Message forwarding: the ability to bounce received messages electronically to other mailboxes.
- f. Subgroup identification, in which a user can identify a group of recipients to receive a message, give the group a single identification name, and address the group with a simple 10-character code.
- g. Archiving of communications: a single floppy disk can store transmitted and received communications for future access.
- h. Gateway to ARPANET (in progress): the ability to communicate

with individuals on a separate network.

- i. Bulletin boards, teleconferencing, meeting preregistration, airline schedules, electronic ordering of IEEE Computer Society publications, and so forth.
- j. Elimination of telephone tag. Messages can be sent and received at a time that is convenient for the user of electronic mail.
- k. Encryption and passwording of messages. Once chemical engineers become familiar with a national chemical engineering electronic mail service, it is quite likely that a number of special interest groups would use it for their rapid communications needs. Typical groups would include, for example:
- Customers of Simulation Sciences Inc.
- Employees of Proctor and Gamble in Cincinnati
- Employees at scattered corporate sites
- Organizers of a conference
- The Editors of and contributors to CAST Communications
- Speakers at CAST Division sessions
- CACHE Board of Trustees
- CACHE Communications Task Force
- CAST executive committee
- Chairman and Heads of Chemical Engineering Departments

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

Given below is an example of a monthly bill for the account, P.RONY,

which he used to transact business as Editor-in-Chief of the IEEE Computer Society magazine, IEEE MICRO. Several messages per day accumulated in his mailbox. Messages were transmitted from disk files, and received messages were stored as one large disk file per session. The modem baud rate was 300 baud.

- 1. Monthly on-line storage, 7.000 blocks at \$0.40 per block = \$2.80
- 2. Prime connect, 1.483 hours at \$10.00 per hour = \$14.83
- 3. Non-prime connect, 1.250 hours at \$4.00 per hour = \$5.00
- 4. Communications/PNET, Prime, 0.200 hours at \$2.00 per hour = \$0.40
- 5. Communications/Telenet, Prime, 1.283 hours at \$6.00 per hour = \$7.70
- 6. Communications/Telenet, Non-prime, 1.250 hours at \$2.00 per hour = \$2.50

Total Bill for November 1984: \$33.23

Clearly, the way to minimize charges is to do all communications at non-prime hours (something which is impossible if a personal computer is not available at home), to have no online storage (delete a message after it is read), and to use a 1200-baud modem. No charge is incurred for a message that remains in a mailbox but is not read.

The CACHE National Electronic Mail experiment has started with a single general account, CACHE, and thirtynine individual accounts,

Y.ARKUN G.BLAU B.CARNAHAN M.CUTLIP M.DAVIS M.DENN T.EDGAR B.FINLAY S.FOGLER I.GROSS J.HALE Yaman Arkun
Gary Blau
Bruce Carnahan
Mike Cutlip
Mark Davis
Morton Denn
Tom Edgar
Bruce Finlayson
Scott Fogler
Ignacio Grossman
John Hale

E.HENLEY Ernie Henley David Himmelblau D.HIMMEL R.HUGHES Richard Hughes R.MAH Richard Mah T.MCAVOY Tom McAvov Duncan Mellichamp D.MELLI Peter K. Mercure K.MERCURE Manfred Morari M.MORARI R.MOTARD Rudy Motard H.PREISIG Heinz Preisig Norman Rawson N.RAWSON Rex Reklaitis R.REKLAIT I.RINARD Irven Rinard **D.RIPPIN** David Rippin P.RONY Peter Rony Ed Rosen E.ROSEN Stan Sandler S.SANDLER B.SEAD J. D. Seader D.SEBORG Dale Seborg W.SEIDER Warren Seider John Seinfeld J.SEINFELD J.SIROLA Jeff Siirola **D.SPRIGGS** Dennis Spriggs George Stephanopoulos **G.STEPH** M.TAYYAB Mike Tayyabkhan Lou Tichacek L.TICHACEK A.WESTBERG Art Westerberg J.WRIGHT Joe Wright

which include members of the CACHE Board of Trustees and officers of the AIChE CAST Division.

CAST Division members are invited to participate in our experiment—which will last for at least six months—at their own expense. For further details, please contact Peter R. Rony at the Department of Chemical Engineering, University of Delaware, Newark, DE 19716, (302) 368-5580, until June 10, 1985, or at Virginia Tech thereafter, (703) 961-7658.

In the hope that some of you will participate, we present the following instructions. System anduser responses are in italics. Further details available in the are COMPMAIL+ manual that is provided once you become a user. You must obtain a modem (1200 baud preferred) and must know how to make your modem work (typical modem driver software carries the name

KERMIT, SMARTTERM 100, 125, etc.). The best software package is one that permits you to easily upload and download files between your disk and COMPMAIL+. The instructions are given below for TELENET. We have been experimenting with TYMNET and conclude that it offers electronic transmission services that are less subject to noise and message garbling than TELENET. The TYMNET and TELENET (or DATAPAC, in Canada) phone numbers in a city near you can be obtained locally.

- 1. Look in the telephone directory for the TELENET number in your community. If you cannot find one, call Peter Rony. Try looking it up first, however; it should be there.
- 2. Get on your computer and execute the software that drives your modem.
- 3. You should set the baud rate to 1200 (preferred) or 300 (if you must).
- 4. Call the appropriate TELENET number through your modem.
- 5. Type the carriage return (CR) key twice, and then (after you see TERMINAL=) type CR again. When you see the response, type \dot{C} 301 364 and a CR. This indicates that you desire node 364 in Maryland (area code 301), which is the ITT Dialcom node.
- 6. The system will indicate that you have connected. It will ask you to input your identification number. Respond with the following line:

id cmpyyyy xxxx

followed by a CR, yyyy is your identification number and xxxx is your four-letter password; you can obtain both from Peter Rony. If you are successful with the login process to COMPMAIL+, it will be obvious.

- 7. Get into the electronic mail system with the response *MAIL*. Get out of the system with the response *QUIT*.
- 8. Try scanning the contents of your mailbox first with the response *SCAN* or with the response *QSCAN* (for quickscan).
- 9. Next, find out the options of the mail system with HELP or?. If you can store the information

as a file or dump the screen to your local printer, do so while you read the *HELP* file. It is not too long, maybe a couple of pages.

- 10. If you try any of the options, like dumping the ID directory, you had better know how to make the system stop the nearly infinite output that it will give you. Try *ctrl-P* for panic.
- 11. Read the items of interest in your mailbox with READ. When you encounter the -More-response, type a CR. The HELP system will tell you how to qualify what you read, how you can respond to it (for example, REPLY and FORWARD), and how to dispose of unwanted messages (DELETE). Do dispose of most messages when asked (Disposition:) with the D or DEL command. It is good practice to get your read messages out of the system; it also saves money since CACHE and other users are charged heavily for the storage of previously read messages.
- 12. Next, try SEND. Send a message to yourself to make certain that you understand the mechanics. The necessary information that is difficult to find is how to get the computer to send the message, once you have composed it. The correct procedure is a CR followed by a SEND and another CR (the abbreviated command S is also acceptable).
- 13. To get out of the mail system, type QUIT.
- 14. Once out of the mail system, but while you are still on COMPMAIL+, you can issue the HELP command to inspect other things beside the mail system that are available to you. One capability that you may wish to use immediately is the PASSWD command to change your password. Then nobody can spy on you! Other services (airline schedules, news wires, etc.) are costly and should not be used by anyone whose costs are being borne by CACHE.
- 15. Finally, to get off the computer system after QUITting the mail system, issue the OFF command. You will be automatically disconnected from the 301 364 TELENET node.
- 16. Now you are back on your own. Somehow hang up the phone and get out of your modem software gracefully.

Good luck. Let us know when you succeed by sending P.RONY or A.WESTBERG a message. We suggest that you look at your mailbox no less frequently than once a week (the time required for half a turnaround using our nation's distinguished non-electronic mail service). Identify a colleague and initiate a regular exchange with him. To minimize costs, send and receive messages after 7:00 PM and before 8:00 AM. Off-hour COMPMAIL + rates are one-third the normal rates.

If you plan to use TYMNET, then modify steps 4 and 5 as follows:

- 4'. Call the appropriate TYMNET number through your modem.
- 5'. When you see the response CONNECT type a CR. When you see the message, please type your terminal identifier: type a lower case a only (no carriage return). When you see the message, please login:, type DIALCOM;64 followed by a CR.

If you are accessing the system from Canada you must go through the DATAPAC system. Modify steps 4 and 5 as follows:

- 4". Call the appropriate DATAPAC number through your modem. Respond to the indication of a connected line (the modem detests a carrier) with .CR or ..CR for 300or 1200-baud, respectively.
- 5". The system will respond with DATAPAC:
 ####### indicating the local access
 point. Type P 1311030100364 followed by a
 CR.

NOTE: Most of the above material appeared in the September 1984 and April 1985 CACHE Newsletter, which is mailed to academic chemical engineering departments worldwide.

Microcomputer/Personal Computer Notes

Edited by Peter R. Rony, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061

The CACHE Newsletter has a regular department that is patterned after *Heart Cut* in Chemtech magazine (published by the American Chemical Society). Given below are selected

items from the spring 1985 Newsletter. If you find this type of material interesting, please let the Editor know. We welcome contributions to these Notes.

Summary evaluations of leading business computer programs and a listing of the most popular applications software are contained on pages 117-124 of the December 1984 issue of Business Computer Systems, which is circulated without charge to qualified subscribers (Cahners Publishing Company, 221 Columbus Ave., Boston. MA 02116). TK!Solver is the fifth largest selling spreadsheet, after Multiplan, FlashCalc, VisiCalc, and SuperCalc3. Bank Street Writer and PFS:Write are the top two word processors. Popular packages in the miscellaneous category are Dollars and Sense, Chart, Sensible Speller, Microsoft Project. SpellStar. PFS:Proof, Harvard Project Manager, and Desk Organizer.

Byte's special issue on communications (December 1984) features articles on "The Evolution of a Standard Ethernet," "Local-Area Networks for the IBM PC," "High-Speed Dial-Up Modems," "Writing Communications in BASIC," "Looking for the Perfect [Communications] Program," and "The On-Line Search."

The February 1985 issue of Byte (page 42) contained a short announcement that caught our fancy: "Satellite Broadcast Network has announced a satellite service that will transmit financial and news information to personal computer owners. You will 12-GHzneedasatellite-receive antenna, a low-noise amplifier, a solidstate receiver, and SBN's demodulator: all are available from SBN for \$695. SBN will also charge a fee for access to each type of information, starting at about \$25 per month. SBN will use multiple 9600-bps channels." Contact Satellite Business Network, Inc., 212 West Superior St., Chicago, IL 60610. The low cost for the antenna and

associated hardware indicates that this type of technology will impact all of us before too long.

"DEC Puts VAX on Eight ICs" (Datamation, February 1, 1985) predicts that a desktop version of the 11/780 supermini is coming from DEC next year, with a price that is 70% less. "But the ink was hardly dry on the MicroVAX II before talk emerged of a 1.22 million-transistor/chip MicroVAX III, allegedly already in silicon. . . The MicroVAX III is believed to have an I/O capability equal to DEC's line-topping Venus, some 13.3 MBps." DEC has been having a rough time in the competitive personal computer market lately.

APL*PLUS/PC (Version 3.1)is reviewed in the January 1985 issue of Dr. Dobb's Journal. The review mentions an excellent comparison between APL*PLUS/PC (Version 2.6) and IBM APL (Version 1.00) that appeared in the March 1984 issue of Byte. Also reviewed or discussed in this issue are VSI-Virtual Screen Interface (Version 2.09), which "is a programmer's tool kit for building applications that manipulate the PC's screen to take advantage of overlapping windows and features such as color and borders," and PCDOS (Version 3.0). The February 1985 issue of Dr. Dobb's reviews Modula-2/86 (Version 1.04).

In Electronics Week (December 10, 1984), Sytek Corp.'s move to license PC Network protocols is discussed. PC Network is based on Sytek's Local 20, "a product that is a carrier-sense, multiple-access, local-network system with collision detection operating at 2 MB/s on coaxial cable. IBM licensed the protocols from Sytek for use with PC Network." "For \$5000, Sytek will license the description of its protocols and the protocol specifications with which other firms will be able to build products that would be compatible with IBM's network . . . ". IBM's objective is to dominate the local network market

as it does the personal computer market. An important competitor is Ethernet, which currently has 2000 installations.

The December 17, 1985 issue of Electronics Week continues its attention to local area networks (LANs) with two brief discussions, "Two Low-Speed Nets Race to Link Computers" and "Unique Net Links MACs with IBM PCs." The first is on AT&T's 1-Mb/s and 2-Mb/s local-area which are vying networks, selection by the IEEE as standard for personal computers. The second is on Transcendental Networking System, which can link computers of different makes and operating systems, such as the IBM PC, Apple Macintosh, and UNIX- and CP/Moriented microcomputers; networking system is known as Tops. The dust should settle in the LAN area within several years.

A significant product announcement appeared in the February 11, 1985 issue of Electronics Week. "Super Cube," which is based upon the Caltech Cosmic Cube, now becomes Intel's 'personal supercomputer' and brings megaflops-range processing within reach of more individuals. Called the iPSC, the product contains 32, 64, or 128 nodes, each node containing an 80286 CPU, 80287 math coprocessor, 512-Kbytes of CMOS DRAM, and 64-Kbytes of ROM. Interested? Prices are expected to range from \$150,000 to \$500,000. When one considers the history of how prices of computer hardware decrease. 2.5 to 10 Mflops of computing power should be on your desktop by 1990 for under \$20,000 (1990 dollars).

"LAN"willchipssoonrivalmicroprocessors instrategic importance," says Dave House, vicepresident of Intel Corporation (Electronics Week, February 11, 1985, 26-27). "House savs microprocessors are running out of gas in terms of complexity, and that the 32bit design is likely to prove to be a practical limit. Even the Cray Systems Inc. supercomputer, he points out, uses a 32-bit instruction. The next level of growth will come from tying personal computers together, so that we go from making individuals more productive to making organizations more productive, House says." We agree. If the 1970s can be considered to be the decade of the personal computer, then the 1980s will be considered as the decade of the computer network.

An important new product is the Intel 27916 KEPROM, which is described on page 73 of Electronics Week (February 11, 1985). What is a KEPROM? It is a Keyed-access erasable programmable read-only memory; it is used to prevent unauthorized copying of ROMstored system software. "Gaining access to stored code in a system that contains a 27916 KYPROM entails an authentication handshake procedure. Thehandshakerequires KEPROMs to communicate with each other-over telephone lines or directly bus on α processor aboard-according to atwo-way verification protocol." The handshake routine is as follows: "1. KEPROM 2 generates random number. 2. Random number is written to KEPROM 1. 3. KEPROM 1 encrypts number. 4. Encrypted number is written KEPROM 2. 5. KEPROM 2 compares this value with original random 6. If there is a match, number. KEPROMs reverse roles and repeat handshake routine."

IEEE Spectrum (January 1985) is a special issue on Technology Experts review developments in minis and mainframes, personal computers, software, microprocessors, communications, solid state, instrumentation, industrial electronics, power and energy, consumer electronics. transportation, aerospace and military, and medical electronics.

The December 1984 issue of Mini-Micro Systems has a number of

interesting brief articles. For example: (a) On page 37, it is stated that "IBM PCs now are the leading resident on engineers' desktops." According to Dr. Joel N. Orr, "The PCs are cheap compared with Digital Equipment Corp. and Hewlett-Packard Co. products, and they are ubiquitous." Two articles briefly discuss different **IBM** PC Engineering/Scientific (PC/ES) workstations. (b) Digital Inc. Research. will market Macintosh-like interface to MS-DOS. It is called the Graphics Environment Manager (GEM), which replaces MS-DOS commands and utilities by icons such as disks and trash cans and by pull-down menus. Companion software products include the GEM Desktop, GEM Programmer's Toolkit, GEM Draw, and GEM Wordchart. The products should appear sometime in "New DECmate and 1985. (c) Computers Receive ProfessionalWelcome" 54-59) Lukewarm (pp. discusses the problems that DEC is having at the low end of its computer (d) "Third-party Developers Concerned Over IBM Microcomputer Software" (pp. 62-63) has a lovely figure that summarizes "IBM's 31 flavors of software." (e) "Will IBM Personal Computers Set a New Hardware Bus Standard" (page 75). The bottom line seems to be as follows: "With IBM's market power and its complete control over the operating CPUsystem, andmother boardconfiguration, the computer industry may find itself endorsing one of the few standards not subject to any standardssetting group's approval." In the world of IBM, seemingly nothing changes. (f) "Operating Systems Conform Application Needs." A nice article by James F. Ready (Hunter & Ready. Inc.) who knows this subject inside and out. Sidebars discuss how operating systems handle application tasks, and how semaphores, mailboxes, monitors prevent resource contention. (g) "Protocol Converters LinkIncompatible Devices." NOTE: Mini-Micro Systems is circulated without

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charge to qualified readers. Write to Cahners Publishing Company, 221 Columbus Avenue, Boston, MA 02116.

The January 1985 issue of Mini-Micro contains Systems the following articles: (a) "Enhancement Programs Add Features to IBM PC Operating System. Application Software." Discusses shell packages-which provide an envelope (or sleeve) around the operating system-and application "Network add-ons. (b) Software Bridges Gap Between Local Area Networks." Novell Inc.'s NetWare fileserver operating system has been ported to 18 major LANs for IBM PC/XTs, ATs, and compatibles. The LANs include Omninet, ARCnet, G-Net, S-Net, proNET, PLAN 2000, EtherLink, PCnet, and MultiLink. Such LANs indicate the degree of competition (and confusion) that currently exists in the area. conservative strategy would involve the selection of a LAN, a standard, from a company that is likely to remain in the field after the dust settles. (c) "Printer Manufacturers Elbow for Shelf Space." Discussion of what is happening in the printer market.

In the February 1985 issue of Mini-Micro Systems: (a) "Networks 1.0 Provides IBMCompatibility." Networks 1.0 is Microsoft's new software that is compatible with IBM's networking scheme. The software runs under the new MS-DOS 3.1 operating system. Microsoft claims it will also run under IBM's PC-DOS 3.1, expected to be available the first (b) "UNIX Emerges as a quarter. Universal Tool Kit" (pp. 149-175). A useful article that includes an extensive directory \mathbf{of} operating system.

From PC World magazine comes the following articles: (a) "Six Leading LANs" (February 1985, pp. 108-128). The networks that are compared include Netware/S-Net, EtherSeries, Omninet, PLAN 3000, PCnet, and

Net/One. (b) "Word Processing: The Deciding Factors" (March 1985, pp. 53-57). The article states: "More than 200 word processing programs crowd the market. Some are easy to use but limited in functions; others can do almost anything but take weeks to master."

The December 1984 issue of Systems Software discusses the IBM XT/370 in "XT 370 Pushes IBM Plan to Link All Products Via VM/CMS" (pp. 63-66).

The Newsletter Format Option

A Report for the CAST Executive Committee May 22, 1984

Charlotte Guthrie, UCCEL Corporation, 1930 Hi Line Drive, Dallas, TX 75297

Sample Layout

The attached layout applies a popular contemporary format to the subjects we have traditionally covered and allows for additional sections proposed earlier by the Publications Board Chairman.

A two-colour, 8 1/2" x 11", three-column, saddlestitch magazine format is proposed. This will easily accommodate 30 to 50 printed pages.

Discussion of Section Contents

Editorial Notes. Review of contents of the issue (alternative: "This ISSUE").

CAST Executive Committee. Listed inside the cover page, along with reports on their activities.

Feature Article. Single theme article for the issue on a topic of general interest to a majority of CAST members.

Feature Events. Reviews of past and future major events (CAST Sessions or FOCAPD). The Programming Board

would contribute heavily to this section.

Articles. Several articles, written for this newsletter or possibly reprinted from other sources, to address a variety of interests, including:

- Microcomputing
- Programmable Calculators
- New Software Products
- All Programming Areas of CAST
- CAST Awards

New Publications. List new books and journals available through AIChE (or elsewhere) which are of interest to CAST members. This large section would contain two major subheadings: Book Reviews and Condensations.

Feature Institutions. News items or summaries of CAST-related university research programs (Ph.D. dissertations and M.S. theses they produce may be reported here or under Publications).

Capsules. Short Articles on non-AIChE CAST-related activities, user groups and other cooperative ventures, announcements or abstracts of news items or articles published elsewhere.

Meetings, Meetings, Meetings. The calendar of activities.

Questionnaires. Surveys can be on the last page for easy removal.

Forum

Artifical intelligence is a rapidly evolving computer technology that is being used or researched in many other engineering fields. I would like to see more sessions at AIChE meetings so that chemical engineers could find out about this area, and those already working in the area could share their results. It would seem that AI would be quite useful in process control applications such as analyzing alarms from a distributed control system, fault tolerance analysis, large scale system designs and many other fields.

Andy Hrymak McMaster University

Your question and request is timely. Note in the CAST Division programming that two sessions are planned for the Chicago Meeting in November to be chaired by Jeff Siirola. We expect that if there is sufficient interest more sessions will appear in the future.

Editor

Meetings and Conferences

following items summarize information in the hands of the Editor by the end of March. Abstracts of presentations at the Houston Meeting (which are given in the meeting catalog) will not be repeated in this Issue in order to provide space for an extra article. By the fall of 1985, we hope that up-to-date programming information will be available on a CAST Division electronic bulletin board. Please send CAST Division session information and meeting announcements to me by August 1, 1985, in time for inclusion in the fall CAST Communications, which will be in our Division members hands prior to the Chicago AIChE meeting.

Editor, CAST Communications

HOUSTON AICHE MEETING (March 24-28, 1985)

Area 10a Sessions

- 1. Plant Retrofitting. I and II, H. Dennis Spriggs (Chairman), Union Carbide Corporation, P. O. Box 8361, South Charleston, WV 25303, (304) 747-7000.
- 2. Process Modeling with Computers- Data Management Aspects. William S. Alper (Chairman), Flour Engineers, Inc., One Fluor Drive, Sugar Land, TX

77478, (714) 263-2111. Robert A. Barneson (Vice-Chairman).

- 3. Process Modeling with Computers- Computational Tools. W. S. Alper (Chairman), Robert A. Barneson (Vice-Chairman), Simulation Sciences, Inc., 1051 West Bastanchury Road, Fullerton, CA 92633, (800) 854-3198.
- 4. Plant Process Information Systems. Donald E. Cormack (Chairman), Setpoint, Inc., 950 Threadneedle, Suite 200, Houston, TX 77079, (713) 496-3220. Gerald A. Hickman (Co-Chairman).

Area 10b Sessions

- 5. Control, Scheduling, and Optimization of Batch Processes. H. F. Boxenhardt (Chairman), Fischer & Porter Co., East County Line Road, Warminster, PA 28974, (215) 674-6086.
- 6. Process Control for Energy Conservation. Richard Weber (Chairman), Exxon Chemicals Americas, Baytown Olefins Plant, P. O. Box 100, Baytown, TX 77520, (713) 428-6385. Ali Cinar (Vice-Chairman).

Area 10c Sessions

- 7. Computing Techniques Review. G. V. Reklaitis (Chairman), Department of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089. Edward Rosen (Vice-Chairman).
- 8. User-Friendliness. Henry L. Bauni, Jr. (Chairman), Exxon Corporation, 180 Park Avenue, Florham Park, NJ 07932, (201) 765-7167. David J. Hersh (Co-Chairman).
- 9. Moving and Organizing Data. T.L. Leininger (Chairman), Computer-Aided Engineering Associates, Inc., 3 Tufts Lane, Newark, DE 19711, (302) 731-4314.

Area 10c Announcement by G. V. Reklaitis

Plans for an Area 10c sponsored oneweek conference: The objectives and subject areas for a one-week FOCAPDstyle meeting entitled "Foundations of Computer-Aided Process Operations," were discussed. The Area 10c Committee approved the plan presented by Dennis Spriggs. The plan also has been approved by the CAST Executive Committee. The Division President will request that CACHE serve as managing agent for the meeting, to be held in the Summer of 1987.

I am terminating my duties as Chairman of the Area 10c Committee. Chairmanship is assumed by Norm Rawson, with Ignacio Grossman as Vice-Chairman. I would like to thank the members of the Committee for their help and support of 10c activities during the past several years.

The Program Committee Meeting of Area 10c, Computers in Management and Information Processing, will meet in Houston, Texas. Anyone interested in joining the Committee or sitting in on the meeting is welcome. Some of the topic areas for which Area 10c has sponsored sessions Technology Reviews, Microcomputers, Data Bases, Workstations, User-Friendly Interfaces, Optimization, Production Scheduling, and other topics of computer applications that do not directly fall into either Area 10a (Systems and Process Design) or Area 10b (Systems and Process Control). The Committee would like encourage your participation and ideas.

Norman E. Rawson (Chairman), IBM Corporation, Dept. 83V, 6901 Rockledge Drive, Bethesda, MD 20817. (301) 564-5959.

USE OF COMPUTERS IN CHEMICAL ENGINEERING, CAMBRIDGE, ENGLAND (March 31 to April 4, 1985)

This conference was organized by the Institution of Chemical Engineers on behalf of the European Federation of Chemical Engineering. More information is available in the December 1984 Issue (Vol. 7, No. 2) of the CAST Newsletter.

AMERICAN CONTROL CONFER-ENCE, BOSTON (June 19-20, 1985)

AICHE is one of the five sponsoring societies for this annual conference. Tom McAvoy, University of Maryland, (301) 454-4593 is coordinator for the nine AIChE sessions at this conference. Irv Rinard, Halcon SD Inc., Two Park Avenue, New York, NY 10016 becomes the AIChE director of the American Automatic Control Council. replacing Alan Foss. University of California at Berkeley.

SEATTLE AICHE MEETING (August 1985)

No CAST Division sessions are planned.

CANADIAN SOCIETY OF CHEMICAL ENGINEERS MEETING, CALGARY (October 6-9, 1985)

Two sessions on Process Dynamics and Control, Dale Seborg (Co-Chairman), (805) 961-3352, J.D. Wright (Co-Chairman), (416) 823-7091.

2-4 sessions on Microcomputer Applications.

CHICAGO AICHE MEETING (November 10-15, 1985)

Area 10a Sessions

1. Interface Between Design and Control (co-sponsored with Area 10b). J. M. Douglas (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2252.

- Manfred Morari (Vice-Chairman), Department of Chemical Engineering, University of California, Pasadena, CA 91125.
- 2. Computers in Process Design and Analysis (2 sessions). Gary Blau (Co-Chairman), Dow Chemicals, Bldg. 1707, Midland, MI 48640, (517) 636-5170. Larry Biegler (Co-Chairman), Department of Chemical Engineering, Carnegie-Mellon University, Pittsburg, PA 15213, (412) 578-2232.
- 3. Applied Mathematics. Vladimir Hlavacek, Department of Chemical Engineering, State University of New York, Buffalo, NY 14260, (716) 636-2910. John C. Haydweillger (Vice-Chairman), Department of Chemical Engineering, University of Syracuse, Syracuse, NY 13210, (315)423-4468.

Area 10b Sessions

- 4. New Applications in Process Control. Ali Cinar (Chairman), Department of Chemical Engineering, Illinois Institute of Technology, Chicago, IL 60616, (312) 567-3042.
- 5. Advances in Process Control. N. Nazmul Karim (Chairman), Department of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO 80523, (303) 491-7871 or 491-5252.
- 6. Developments in Dynamic Modeling and Simulation. John C. Friedly (Chairman), Department of Chemical Engineering, University of Rochester, Rochester, NY 14627, (716) 275-4041. Mark Juba (Co-Chairman), Kodak, (716) 477-6542.
- 7. Interface Between Design and Control (see Area 10a).

Area 10c Sessions

8. Expert Systems: State-of-the-Art Review. Jeffrey J. Siirola (Chairman), ECD Research Laboratories, Eastman Kodak Co., Kingsport, TN 37662, (615) 229-3053.

- 9. Expert Systems: Applications in the CPI. Jeffrey J. Siirola (Chairman), ECD Research Laboratories, Eastman Kodak Co., Kingsport, TN 37662, (615) 229-3053.
- 10. Progress towards Process Engineers' Station. Edward M. Rosen (Chairman), Monsanto Co., 800 No. Lindbergh Blvd., St. Louis, MO 63167, (314) 694-6412.

CHEMICAL PROCESS CONTROL III, ASILOMAR (January, 1986)

This third conference in the Process Control Series will be held at the Asilomar Conference site in California. The exact date in January 1986 is available from Tom McAvoy, University of Maryland, (301) 454-4593, or from Manfred Morari, Caltech, (818) 356-4186, who are the organizers.

NEW ORLEANS AICHE MEETING (April 6-10, 1986)

The meeting program chairman is Jack R. Hopper, Department of Chemical Engineering, Lamar University, P. O. Box 10053, Beaumont, TX 77710, (409) 838-8784.

Area 10a Sessions

- 1-2. Simulation in Chemical Engineering. Mark A. Kramer (Chairman), Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, (617) 253-6508. Herb Britt (Co-Chairman), Aspen Technology, 251 Vassar Street, Cambridge, MA 02139, (617) 497-9010.
- 3. Industrial Experience with Large Simulators. Chairman to be announced. (See also sessions on Workstations and Data Reconciliation sponsored by 10c).

Area 10b Sessions

1. Process Monitoring and Identification. Fred Ramrirez (Chairman), Department of Chemical

Engineering, University of Colorado, Boulder, CO 80302.

- 2. Advances in Computer Control. Odd Asbjornsen, (Chairman).
- 3. Advances in Process Control. Herman Bozenhart (Chairman).

Area 10c Sessions

- 4. Impact of Microcomputers on Industry and Universities. Norman Rawson (Chairman), IBM Corporation, Dept. 83V, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 564-5959. Brice Carnahan (Co-Chairman), University of Michigan.
- 5. Computer-Aided Engineering. H. Dennis Spriggs (Chairman), Union Carbide Corporation, P. O. Box 8361, South Charleston, WV 25303, (304) 747-7000. Kris R. Kaushik (Co-Chairman), Shell Development Corporation.
- 6. Computer Support of Plant Operations. John Hale (Chairman), E.I. DuPont de Nemours & Co., Louviers Building 3, 56, Wilmington, DE 19898, (302) 366-3041. Iren Suhami (Co-Chairman), Exxon, Florham Park.

CANADIAN INDUSTRIAL COMPUTER SOCIETY MEETING (May, 1986)

About 20 sessions, Jules O'Shea (Technical Program Chairman) Ecole Polytechnique, CP 6079, Succ. "A" Montreal, P.Q., H3C 3A7, (514) 340-4711.

AMERICAN CONTROL CONFERENCE, MINNEAPOLIS (June, 1986)

Professor Yamun Arkun, Renssalaer Polytechnic Institute, (518) 266-6765, takes over responsibility for the AIChE activities in the American Control Conference. This will allow Tom McAvoy, University of Maryland, (301) 454-4593, to handle all Area 10b programming.

BOSTON AICHE MEETING (August 24-27, 1986)

No CAST Division sessions are planned.

MIAMI BEACH AICHE MEETING (November 2-7, 1986)

Area 10a Sessions

- 1-2. Applied Mathematics. Stuart W. Churchill (Chairman), Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 19104, (214) 898-5579.
- in 3-4.Simulation Chemical Engineering. Warren Seider (Chairman), Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 898-7953. 19104, (214)Art Westerberg (Co-Chairman), Department of Chemical Engineering, University, Carnegie-Mellon Pittsburg, PA 15213, (412) 578-2230.
- 5. Synthesis. George Stephanopoulos, (Chairman), Department of Chemical Engineering, Masschusetts Institute of Technology, Cambridge, MA 02139, (617) 253-3904. Rakesh Govind (Vice-Chairman), Department of Chemical Engineering, University of Cincinnati, 697 Rhodes Hall (ML 171), Cincinnati, OH, 45221-0171, (513) 475-2761.
- 6. Perspectives in Computer-Aided Design and Operation. John Perkins (Chairman), Department of Chemical Engineering, Imperial College, London, Prince Consort Road, London, England, SW7 2BY, 01-589-5111.

Area 10b Sessions

1. The Relative Gain Array - A 20 Year Retrospective. Tom MacAvoy (Chairman), Department of Chemical Engineering, University of Maryland, College Park, MD 20740, (301) 454-4593.

- 2. Unsolved Problems in Process Control. Manfred Morari (Chairman), Department of Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, (213) 263-2923.
- 3-4. Recent Advances in Process Control. Joseph Wright (Chairman), Xerox Research Centre of Canada, 2660 Speakman Drive, Mississauga, Ontario, Canada, L5K 2L1, (416) 823-7091.

Area 10c Sessions

- 5. Engineering Issues in Vector Computing. Mark Stadtherr (Chairman), Department of Chemical Engineering, University of Illinois, Urbana, IL 61801, (217) 333-0275.
- 6. Design and Application of Special Purpose Computers and Processing Systems. Peter R. Rony (Chairman), Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061, (703) 961-7658 or 961-6370.

HOUSTON AICHE MEETING (Spring, 1987)

Area 10c Sessions

- 1. Opportunities in the Application of Management and Technical Information Systems.
- 2. Production Scheduling.
- 3. Career Opportunities in Chemical Engineering Computing.
- 4. Cost/Benefit Assessment of New Computing of Technology (Panel).

FOUNDATIONS OF COMPUTER-AIDED PROCESS OPERATIONS (Summer 1987)

Area 10c is planning to hold this conference, which will be patterned after the highly successful "Foundations of Computer-Aided Process Design" (FOCAPD) series, but emphasis with much more industrial aspects of computer applications.

AICHE MEETING (Fall, 1987)

Area 10c Sessions

- 1. Large Scale Optimization.
- 2. Intelligent Processing (Manufacturing) Systems.

SIMSCI'S INPUT+, InterFlash, & PIPEPHASE

Petty Tremblador, Simulation Sciences Inc., 1051 W. Bastanchury Road, Fullerton, CA 92633, (714) 879-9180

N. Fred Brannock, Vice-President of Simulation Sciences, Inc. announces the release of three new products: (1) INPUT+ the first-in-a-family of PC/PROCESS products, (2) InterFlash, and (3) PIPEPHASE.

INPUT+ allows the user to prepare PROCESS input on an IBM PC or compatible desktop without logging onto a mainframe. The help facilities bring a higher level of efficiency to even a novice user.

The INPUT+ basic tutorial approach and comprehensive HELP facilities allow users to teach themselves how to prepare PROCESS input. Special features of INPUT+ include: full screen editor and on-line keyword HELP, 1000+ PROCESS chemical data bank library of names, on-screen PROCESS manual, single-stroke load templates, built-in specification templates, and single-stroke input checks.

PC/PROCESS brings you the power and comprehensive capabilities of the PROCESS simulation program on your personal computer. INPUT+ is the first in a growing family of special-purpose programs derived from PROCESS and designed to take full advantage of the user-friendly features and convenience of the microcomputer. Each program in the PC/PROCESS Family will be compatible and consistent with PROCESS and will

maintain the same high standard of comprehensiveness and quality.

InterFlash gives the user interactive access to all the vast flash calculations and properties prediction capabilities of PROCESS, but in a smaller, more convenient program. Output is readymade to provide easy-to-read tables and plot displays on your CRT screen or printout.

InterFlash contains all of the industry standard methods and data for predicting properties available in PROCESS, including its data bank of over 1000 pure components, full complement of physical, thermodynamic and transport properties, and full-capability petroleum assav handling and characterization procedures. InterFlash versions are available for IBM, DEC-VAX, and Prime computers.

PIPEPHASE is a comprehensive steady-state, single-phase, or multiphase fluid flow piping network simulator that efficiently solves any type of piping problem from a simple pipe to a complete network, including gathering and distribution systems. The strength of PIPEPHASE stems from the successful integration of industry standard PVT properties packages, comprehensive pure component library, and oil assaying procedures.

PIPEPHASE can be used both to design new piping systems and facilities and to simulate and optimize performance of existing systems. Areas of applications include: oil field applications, oil and gas transmission and process plants—refining and petrochemical. PIPEPHASE employs easy-to-use, free format input. Output is professionally presented in well designed tables and printer plots. The properties packages available in PIPEPHASE include all of those applicable from SIMSCI's PROCESS simulation program.

Proceedings of the Second International Conference on "Foundations of Computer Aided Process Design" (FOCAPD)

Edited by Arthur Westerberg and Henry Chien

Proceedings of the FOCAPD held conference at Snowmass. Colorado in the summer of 1983 are now available. The week long meeting, featuring papers by leading academic and industrial researchers in the computer-aided design field, was sponsored jointly by the CAST Division of the AIChE and CACHE, with support from the National Science Foundation and nine corporations corporate and foundations including: Chivoda Engineers and Construction Co., EXXON Research and Development Co., the Halcon SD Group, Monsanto Company, Olin Chemicals Corp., Simulation Process International, Shell Companies Foundation. Tennessee Eastman Co., and Wyerhauser Co.

The Proceedings (a hardbound book of 1042 pages) contains all 22 papers presented during the meeting, plus summaries of the discussions held during each session.

The titles of the major sessions were:

FOCAPD Proceedings Papers:

Expert Systems and Technological Problems, by P. E. Hart

Discussion Summary of Keynote Address, by A. W. Westerberg

Process Systems Engineering-Challenges and Constraints in Computer Science and Technology, by R. W. H. Sargent

Challenges and Constraints in Computer Implementation and Applications, by S. I. Proctor

Discussion Summary of Overview and Outlook, by J. L. Robertson

The Database Frontier in Process Design, by P Winter and C. J. Angus

Database Technology Applied to Engineering Data, by R. M. Balza, D. L. Bernhardt, and R. P. Dube

Relational Databases for Engineering Data, by R. Lorie and W. Plouffe

Discussion Summary of Progress in Database Development, by T. L. Leininger

Model and Algorithm Synthesis in Process Analysis and Design, by W. D. Seider

Discussion Summary of Computational Algorithms, by G. E. Blau

Structure of Thermodynamics in Process Calculations, by J. P. O'Connell

Efficient Use of Thermodynamic Models in Process Calculations, by E. A. Grens II

Equation-Based Flowsheeting, by J. D. Perkins

Simultaneous Modular Simulation and Optimization, by L. T. Biegler

Discussion Summary of Nonsequential Modular Flowsheeting, by E. Gordon and K. O. Simpson

Discussion Summary of Nonsequential Modular Flowsheeting, by V. Hlavacek

Discussion Summary of Nonsequential Modular Flowsheeting, by R. L. Motard

Intermediate Storage in Non-Continuous Processing, by I. A. Karimi and G. V. Reklaitis

On the Design and Analysis of Efficient Algorithms for Deterministic Scheduling, by H. N. Gabow

Discussion Summary of Design and Scheduling of Batch Chemical Plants, by R. S. H. Mah

Collocation Methods in Distillation, by W. E. Stewart, K. L. Levien, and M. Morari

Computer Modeling of Chemical Process Reactors, by H. H. Klein

Discussion Summary of Complex Single Unit Design, by B. A. Finlayson and B. Joseph Scheduling of Multipurpose Batch Plants with Product Precedence Constraints, by I. Suhami and R. S. H. Mah

The Prediction of Properties and Its Influence on the Design and Modeling of Superfactionators, by M. R. Hernandez, R. Gani, J. A. Romagnoli and E. A. Brignole

Low-Cost Solutions to Multistage, Multicomponent Separation Problems by a Hybrid Fast-Point Algorithm, by A. Lucia and K. R. Westman

Solutions of Systems of Interlinked Distillation Columns by Differential Homotopy-Continuation Method, by T. L. Wayburn and J. D. Seader

Strategies for Simultaneous-Modular Flowsheeting and Optimization, by M. A. Stadtherr and H. S. Chen

Recent Developments in Solution Techniques for Systems of Nonlinear Equations, by M. Shacham

Discussion Summary of Contributed Papers, by C. M. Crowe

Operability, Resiliency, and Flexibility-Process Design Objectives for a Changing World, by I. E. Grossman and M. Morari

Discussion Summary of Operability in Design, by J. M. Douglas

Discussion Summary of Operability in Design, by I. H. Rinard

Discussion Summary of Operability in Design, by G. Stephanopoulos

The text is available at \$37.50 from Professor Brice Carnahan, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109.

"Make Your Wish Upon a Star"

Or How this Issue was Developed

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At the AIChE meeting in San Francisco last November, the CACHE Board of Trustees, including the Editor of CAST Communications was invited to visit the Xerox Palo Alto Research Center. During the visit, the Xerox 8010 Star System software was demonstrated along with a number of other recent developments in Interlisp-D, artificial intelligence applications, and so on. Your Editor was so excited that he spent the next two or three days mumbling to himself variations on a theme of . . "I wish I had a Star", to various well-known tunes from Disneyland Productions, and . . . " why can't I have one of those?" His return to reality forced him to take a different tack which was to convince certain contacts he had at Xerox to collaborate with him on his new venture as Editor of CAST Communications.

As part of the new Communications adventure, we agreed to assemble the entire package by making use of the CACHE Corporation Electronic Mail Experiment. All of the articles and files were to be collected by the Editor on his computer in Delaware and then transferred to a Star System at the Xerox Research Centre of Canada. Questions related to CAST Communications would be discussed using the electronic mail system, as described elsewhere in this Issue and files would be transferred electronically as they were developed. Final formatting and preparation of the camera-ready copy was to be carried out on the Star System.

The use of electronic mail to transfer documents is relatively well accepted within many Corporations and is

common in some engineering disciplines. Use in the chemical engineering community is less well established and so a number of interesting hurdles had to be overcome as we proceeded with our experiment. The first problem which encountered was how to access either TELENET or. TYMNET through which we eventually accessed the COMPMAIL+ system from Canada. The problem was that there was no listing for TELENET or TYMNET in the Mississauga or Toronto telephone directories. Internal information at Xerox identified a DATAPAC number and account, but all attempts to use these resulted in an automatic connection with the Xerox Computer Center in Rochester. We eventually acquired the correct account number which would connect DATAPAC directly to COMPMAIL+ the computer system by calling ITT DIALCOM and asking for help. (This number is shown for Canadian users in the article on Electronic Mail.)

Once we were able to access the COMPMAIL+ service, it was possible to exchange messages with Peter Rony and to determine the next step in the process. We found that it was not obvious how to transmit files in an elegant way. Commercial modem control packages for use on home computers usually have commands to transfer a file from one machine to the modem lines and hence potentially to another computer elsewhere. However, COMPMAIL+ service did not appear to be easily adaptable to this simple process. Our solution was to use the CHAT mode of communications and transfer files from the Editor's computer to the Star system as if in a CHAT mode. At the Star end, the files were captured and placed in a contiguous disk file. This file. incidentally, contained all of the CHAT dialogue as well as the files themselves. A minor problem which arose and which will be discussed later on was that the CHAT buffer size is only 120 characters long. That meant we had to insert frequent carriage returns. In practice this turned out to be at the end of every line.

The contents of this Issue transmitted in approximately sessions, some of which lasted more than an hour. We were restricted at both ends, unfortunately, to 300 baud modems. 1200 baud would have been a preferred option. During the transfer these various files we had occasional glitches in the system which caused loss of communications and necessitated re-transmission of some of the files. We also found that the use of CHAT mode meant that the end-of-file protocol was not handled as cleanly as it is with packages designed for file transfer. The result was that extraneous characters and messages often appeared at the end of each major file.

A self-imposed deadline to complete the preliminary editing task prior to the Houston AIChE meeting, so that we could discuss some of the details of the new formatting etc., dictated that we also make use of the electronic mail system through Joe Wright's personal computer at his home in Burlington. DATAPAC was accessed by a local number, which by this time we knew how to find in the telephone directory. We used standard modem control programs to receive the results of the CHAT dialogue. Raw files were stored under CP/M format on a diskette. Subsequently, these were brought to the Research Centre and read into the Star System through its diskette drive. The files were then translated into Star System format and the same procedures were followed, as before.

Transferring the files to the Star System was only the beginning of the rather significant amount of work required to transform a conventional word processing document into what is essentially a typeset equivalent. The Star System assigns properties to special carriage returns which appear at the end of each paragraph. These are different from a normal carriage return and contain information about tab settings, margins, justification, and so on which are important for formatting operations. It was necessary to replace the carriage returns, which were genuine end-ofparagraph (or end-of-major-heading) with Star System paragraph returns. This was easily done with a global substitute command. However, we had to differentiate from conventional returns which appear, for example, at the end of an address, or a tabular entry in the text. As a result, we were forced to adopt a convention to enhance the search. The Editor included ** with each of the end-ofparagraph returns in his files. then substituted all occurrences of **CR with the paragraph return symbol used on the Star System. Although this put in the paragraph returns in the appropriate places, we still had to eliminate the end-of-line returns which appeared throughout the document. A global substitution worked well for normal text. But, in areas where returns were really wanted, e.g., any list of addresses, and in the tables, this command was disastrous. We, therefore, found that a combination of automatic and semiautomatic substitution with confirm was necessary. In retrospect, we could have used some wild card character like a single * for required ordinary CRs and done a similar substitution to the one for paragraph returns. This would have saved considerable formatting time on the Star but would have perhaps increased the editing time on the conventional computer system.

There were other minor character problems to correct. One of these was the use of hyphens in the conventional word processor. This is a standard dash in most systems. The Star system differentiates between an em-dash and

an en-dash. As a result, we did a global substitution for these with confirm as necessary. An interesting problem, which resulted from the choice of fonts for this Issue, was caused by quotation marks. In a printer mode, the quotation marks are identical for both opening and closing quotes (" "); however, in this particular font, which is a Classic font, the opening and closing quotes are different (" "). Again, this meant a global search, but with a considerable amount of manual effort required to insert the changes.

There were a number of issues related to the general style and layout of the Communications Issue. One of them was the font size to be used for final copy. We produced an 8-point type (the size of the small print in this issue) and a 10-point version which we presented in draft form to several of the CAST Division Executives following the Houston AIChE meeting. The decision was that the 10-point type was more readable with smaller font size reserved for detail information in appropriate places. For general layout, we essentially followed the recommendations of the AIChE for newsletter formats. as discussed elsewhere in this Issue. The final result is what you see.

We will not discuss in detail the tremendous amount of work which went into the many iterations on format, standard editing, corrections We very gratefully and revisions. acknowledge the superb effort of Debbie MacPhail who patiently and efficiently implemented our many good and not so good ideas and then fixed up the changes as we changed our minds again. She, too, learned from the electronic mail experiment, sending some messages to Peter Rony on progress and deciphering the CHAT dialogues to find the real content of the Communications. We expect the next Issue will be much more effectively handled as we delegate much of the work and utilize the experience we have gained from the current work.

Proofreading of the Master Copy was done by Chris Wright, in the true spirit of volunteer labour as outlined by our Chairman in his remarks. The final printed camera-ready copy was sent to Barbara Boyer at AIChE Headquarters, where the printing and distribution were handled in the usual efficient way. The results are as you see them and we would certainly be interested in any comments you have on general format, style and content.

Overall, the experiment was tremendous success. We were able to transmit all relevant information electronically, with relatively little difficulty once the general protocols etc. were sorted out. We did find that there was major editing work to be done to translate the low level word processing document into the more sophisticated Star System format. Our learning curve was very steep, but generally we felt the exercise showed great potential and we will be working very hard before the next Issue to the whole streamline operation. Meanwhile, those of you who wish to submit notes, articles, letters to the Editor through the Forum Section etc., are encouraged to communicate all of the information via electronic mail.

Acknowledgment

The CAST Division of AIChE gratefully acknowledges the support of Xerox Corporation and in particular the Xerox Research Centre of Canada for their support in producing this Communications on their 8010 Star Systems.

Editor

CAST Proceedings: A Survey of CAST Division Membership by Peter R. Rony

There are widely divergent views among different segments of AIChE as to their desires regarding publications. These views vary from the desire for peer review of all technical papers to the desire for distribution of hard copies of meeting papers, without peer review, in advance of national meetings. The debate on this issue has been active in recent months within the Fuels and Petrochemicals Division, whose members prefer hardcopy to microfiche. In anticipation of the possibility that this issue will be addressed to all divisions within the AIChE, the CAST Division Executive Committee would like to poll the membership concerning the publication of two volumes of CAST Proceedings per year. The proposal is that all papers presented at CAST Division sessions would be reduced to book size, printed with an inexpensive binding, and distributed to all CAST Division members at an estimated cost in dues of approximately \$16 per year (a cost that also includes two issues of CAST Communications per year). The current annual dues for the CAST Division is \$5. Approximately 120 papers per year are presented at CAST Division sessions, and most of these would be available in the Proceedings, which would be mailed prior to the national meetings. The papers would NOT be reviewed. Refereed journals do not view a paper contained in a proceedings as a publication.

We solicit your guidance on this matter. Please fill out the attached survey and mail it to Ed Rosen, Chairman of the CAST Division. Normally, the response to surveys such as this one is very small. This is an important decision; please take a few minutes of your valuable time to help the CAST Executive Committee learn how best to serve Division Members.

то:	Dr. Edward M. Rosen Monsanto Company CS7C800 No. Lindbergh Blvd. St. Louis, MO 63167	AST Division	Survey		
1.	Would you prefer a Proceedings instead of microfiche?		☐ yes	no no	
2.	Would you be willing to pay an extra \$11 dues for the CAST Proceedings volumes?		☐ yes	no no	
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