TECHNICAL COMPUTATIONAL NEWSLETTER

Sigmund J. Lawrence, Editor

First Quarter, 1977

A COMPUTING TECHNOLOGY DIVISION

A subcommittee consisting of past-chairmen of MCC has been investigating the feasibility of forming an Institute Division to represent the interests of Ch.E.'s in computer applications, mathematical applications, management sciences and control systems. With the appointment of R. L. Morris of ITT Continental Baking Company as Chairman of a Division Formation Committee, the Institute's Council has given this MCC activity official status and a report of activity was made to Council at the Chicago meeting.

A survey of AIChE members who indicate computer applications or process control as their primary professional interest has been completed. 79% of the respondents indicated that they support formation of the proposed Division. 19% had no strong feeling one way or the other and only 2% objected to the Division. 51% of the respondents said they would definitely join the Division. With these people we now have a mailing list of potential members which includes about 1000 names.

A draft set of By-Laws have been prepared and after preliminary review by Council are under final revision by a sub-committee headed by Bob Fisher of Mobil. The document follows very closely the structure of the very successful Environmental Division By-Laws and also borrows heavily from those of the Heat Transfer and Energy Division. A key characteristic of the proposed division structure is the ability to form Sections within the Division to represent specific categories of technical interests. This structure carries over heavily into the programming responsibilities of the Division in order to ensure continuation of the many areas of programming interest presently active in the National Program Committee. Warren Seider of the University of Pennsylvania is preparing the required division formation budget while Vern Sterba and Charlie Ware, chairman and past-chairman of MCC, are drawing up the required operating plan.

Other members of the formation committee include Ted Peterson, Dick Hughes, Mary Ann Epstein, Mike Tayyabkhan, Al Johnson, Herb Owens, Brice Carnahan, Dick Mah, Art Westerberg, Bob Weaver, Manoj Sanghvi, Ted Leininger and Max Lee. AIChE members who are interested in the division and who have not been contacted yet should express their interest by writing to Herb Owens at AIChE headquarters. - by Robert Morris

CODATA - COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY

The CODATA organization was founded in 1966 by the International Council for Scientific Unions (ICSU) with F. D. Rossini as its first president. Originally conceived to concentrate on physics and chemistry it has broadened its scope to include the bio- and geo-sciences. It is currently expanding into areas of special significance to chemical engineering. It is dedicated to improving the quality, reliability and accessibility of data on the properties and behavior of matter. Fifteen major nations comprise its general assembly. In the U.S., The National Bureau of Standards acts as the interface for American participation. Any individual or organization may subscribe to the CODATA BULLETIN by writing to the CODATA Secretariat, 51, Boulevard de Montmorency, 75016 Paris, France. The price is $8.00 per year.

Of special interest to chemical engineering are the Task Groups on Fundamental Constants and the Task Group on Key Values for Thermodynamics. The former published its results as CODATA Bulletin No. 11 in 1973. The latter has published standard enthalpies of formation and entropies at 298.15K in CODATA Bulletins No. 10 (1973) and No. 17 (1976). Beginning in 1978, the publication of International Tables of Thermodynamic Properties is proposed as a continuous dissemination medium.

Another group of interest to MCC is the Task Group on Computer Use whose goal is to foster access to data banks of numerical data by bringing together representatives of automated information handling facilities and services. This group serves as a focal point for encouraging the creation of computer readable data banks and examining the standardization requirements.

Finally, at its fifth biennial conference in Boulder, Colorado in June 1976 there was created a Task Group on Data for Industrial Chemicals whose preliminary goal is the dissemination of critically evaluated property correlations for classes of chemical species and their mixing rules. This effort is chaired by Dr. Arnold Bondi of Shell. -

by Rudy Motard

GAZING AT THE CRYSTAL BALL

Ted Peterson and Mike Tayyabkhan of the MCC have set up a questionnaire to probe what chemical engineering computing will be like in the 1980's. The first edition has been sent out to MCC members.

There are over 70 questions, with up to five different statements gathered under one question. I found this intriguing. The responder is to consider himself being in the year 1986, ten years from now. A choice of "Has", "Is", "Will" or "Will Not" is available. "Has" = Has occurred largely by 1986 (e.g., wide market acceptance). "Is" = Is occurring in 1986 (e.g., products appearing). "Will" = Will occur shortly, up to 1990 (e.g., in development in 1986). "Will Not" = Will not occur in foreseeable future (e.g., feasibility not demonstrated). Questions are not numbered in sequence and responses may include multiple check points.

The following areas have been selected: Computing; Chemistry & Chemical Engineering Design Applications; Process Control; General Data Processing Applications; Education; Hardware; Software; Firmware; Micros; Data Bases; Communications; Distributed Computing; Input/Output; Privacy; Reliability; Regulation; Management.

This is a DELPHI approach, i.e., "Contemplate your navel". There is a delightful challenge, especially in that the statements force one to choose among various ways that the industry may opt. Thus I found myself contradicting myself on the first pass, and changed my mind several times. Then there were areas of ignorance, alas.

All in all, it shows a great deal of creative work by the authors, and they are to be commended. I am looking forward to Round Two. - Editor

FROM NORTH OF THE BORDER

The Canadian member of the MCC is Professor A. I. Johnson, Dean of Engineering Science at the University of Western Ontario. He has undertaken to give us a news item in each of the next several issues of the Newsletter to highlight some of the personnel activities, and facilities in Canadian chemical engineering schools and has started the series with a short description of the operations at Western Ontario.

This University has a Centre for Advanced Technology which is sponsored by the Canadian Department of Industry, Trade and Commerce to assist Canadian industry in the evaluation and application of methodology for computer aided analysis design and control of complex systems. While this Centre is engaged in a range of projects, some of the successful projects undertaken have been concerned with complex recycle systems and with the scheduling of multiproduct plants.

Professor Johnson is currently creating a distributed computing system for such studies incorporating an intelligent computer graphics console which has been developed in Canada by the Bell Northern Research Corporation and the Canadian Department of Public Works. He is particularly interested in establishing correspondence with chemical engineers in industry and government who are concerned with computer aided process analysis and design, particularly with those currently engaged in dynamic systems. The rest of his address is London, Canada, N6A 5B9.

POSTER SESSION IN PROCESS DESIGN & CONTROL

The third AIChE poster session was held at the Chicago meeting. Approximately 130 people attended. In the morning a ten minute overview of each of 8 papers was presented. This was followed by a poster session of 1½ hrs. The afternoon format was similar.

For a poster session, each author prepares a 30" x 40" arrangement of 9 pages containing anything which will reinforce, elucidate, or draw interest (such as figures or briefs of major concepts). Each person has his own little corner and answers questions on an informal basis, as the crowd drifts and stops.

E. M. Rosen chaired the am; D. G. Fisher did the honors for the pm. Evaluation forms were handed out, and turned in by 30 of the attendees. Overall response to the poster session idea seemed favorable. About 8 papers to a poster session seemed about right. Most thought that the poster session gave them more opportunity to gain information than does the standard format. Having a short general overview before the poster session was deemed helpful. Practically all thought the idea was good and should be extended. - by E. M. Rosen

THE FOURTH INTERNATIONAL CONFERENCE ON COMPUTERS IN CHEMICAL RESEARCH AND EDUCATION

The USSR Academy of Sciences has expressed interest in hosting the Fourth International Conference in Novosibirsk, USSR, summer of 1978. A new feature has been suggested, namely an exposition.

The NAS-NRC National Committee for the International Union of Pure and Applied Chemistry has been asked to assume responsibility for what has hitherto been an ad hoc series of conferences now that their viability has been demonstrated.

Proceedings of the first three are available, or about to be published, as follows:

"First Conference on Computers in Chemical Education and Research", 660 pages in two volumes, Vol. 1, PB248880/AS, $9.75 paper copy; Vol. 2, PB248881/AS, $10.50 paper copy; from NTIS, Springfield, VA 22161.

Second International Conference on Computers in Chemical Research and Education, Vols. I, II, III, Elsevier Press.

Third International Conference on Computers in Chemical Research, Education and Technology was held last July in Caracas, Venezuela, and the papers are still being collected. Plenum Press will publish the proceedings. -

by Peter Lykos

COMPUTERS IN CHEMISTRY (DIVISION OF ACS)

COMPception happened at the April, 1974, National ACS meeting in LA. Gestation took two years with birth at the April '76 National ACS Centennial meeting in the Big Apple where the word "probationary" was dropped from COMP's title. COMP is now off and running under its first slate of officers (soon to be replaced). Membership has grown from an initial less than 200 to almost 500. COMPsymposia have become a regular feature at national ACS meetings. In March '77 in New Orleans, a symposium will be held on reaction mechanisms, modelling and computers. In May '77 in Montreal, the subject will be minicomputers and large scale computers. Symposia proceedings are being published in hard-back form. The present officers are:

Peter Lykos, chmn	IIT
Edward C. Olson, chmn elect	Upjohn
Rudolph J. Marcus, secy	Off Nav Res
Wm. Lester Jr., treas	IBM Res

by Peter Lykos

SHARE NO LONGER SO FAIR

SHARE was originally set up for free exchange and dissemination of information pertaining to scientific applications on large IBM computers. As such, it was a rich source of computer routines for chemical engineers; however SHARE has broadened its horizons to the extent that it's now concerned with the mainstream of data processing and is virtually indistinguishable from GUIDE, the organization for data processing on IBM machines. Its value to a chemical engineer has greatly diminished unless his computing interest lies in operating systems, data base management, teleprocessing, distributed processing, new computer languages, or installation management. The once strong projects in applied mathematics, Fortran and applications are now feeble. Graphics is a lively topic but concerned primarily with image processing, medical graphics, computer animation, and graphics related to numerically controlled tool programs. The SHARE library, once a primary source, has been brought up-to-date by throwing out all of the work related to old machines (709, 7090, 7094) -- even though many were in Fortran and the product of SHARE's days of engineering and scientific orientation. - by Ted Leininger

CURRENT ACTIVITIES OF IFIP WG5.2 ON COMPUTER AIDED DESIGN

IFIP WG5.2 on Computer Aided Design has already published one volume Computer Aided Design (North Holland 1973) and will soon publish the proceedings of a Working Conference held in February 1976 in Austin, Texas.

The most recent meeting was held in Visograd, Hungary on September 28, 1976. Work is proceeding in the area of graphics methodology and standards, and preparing working conferences in a number of computer aided design areas through 1981. The current chairman of WG5.2 is

E. A. Warman
R and PD Computer Group
Perkins Engines Co.
Frank Perkins Way
Peterborough
England

CAD parallel sessions will be held at the Trienniel IFIP Congress 8-12 August 1977 in Toronto, Canada. - by E. M. Rosen

FREE SOFTWARE: A FORTRAN ROUTINE ORGANIZER

Once in a great while, in combing through the great wasteland of "free" computer software, one comes across something really useful. Such a find is a "FORTRAN Routine Reorganizer" in the Bureau of Mines Information Circular 8696 (1975). The report describes a computer program designed to aid one in analyzing and understanding unfamiliar FORTRAN programs. The routine reorganizes FORTRAN programs and subprograms by sequentially renumbering the statement numbers, sequentially renumbering and relocating all FORMAT statements, alphabetically reordering all DIMENSIONed and typed variables, and providing a uniform pattern of text spacing.

The program described in the report is written in 100% CDC FORTRAN and should be relatively easy to convert to other FORTRANs (however, it includes some ENCODE/DECODE statements). The report presents a complete FORTRAN listing of the program which also serves to illustrate the program output. The publication has been cataloged in the United States Department of the Interior Library as follows: TN 23.U71 No. 8696 622.06173. The author is Marvin S. Seppanen. - by Vern Sterba

NRCC

The National Resource for Computation in Chemistry is close to becoming a reality. Ever since Harry Shull's proposal was discussed at a national forum and distributed widely by the National Academy of Sciences in 1970, there has been a steady and growing movement toward that goal. The current status is that NSF and ERDA have agreed to cosponsor Phase I of the NRCC if a suitable proposal is received from one of the four ERDA National Science Laboratories which have expressed interest in becoming the site. The proposals are due 5 Dec. 76. The NRCC could begin operation within a calendar year of that date. - by Peter Lykos

NOTES FROM THE MCC ANNUAL REPORT

Present MCC membership is 68, up from 57 a year ago. The meetings at Kansas City, Atlantic City and Chicago were attended by 21, 22, and 24 respectively. MCC officers for 1976 were: Charles H. Ware, Jr., Chairman; Vernon J. Sterba, Vice-Chairman; and Warren D. Seider, Secretary-Treasurer. Vern Sterba has succeeded Charlie Ware as Chairman for 1977. (Editor's note - For 1977, Warren Seider is Vice-Chairman, and Robert J. Lackmeyer is Secretary-Treasurer.)

Warren Seider has been succeeded by Art Westerberg as representative to the National Program Committee, Area 1D and Area 1D chairman. Ted Peterson is Chairman of Group 1 and will be Meeting Program Chairman, Atlanta, Feb., 1978. Eight technical sessions were held in 1976, 7 in computing and one in applied math.

Charlie Ware is now in charge of the review of computer programs and their description, to appear in the new journal Computers and Chemical Engineering. Coleman Brosilow is now Liaison Coordinator. Rudy Motard has been coordinating the efforts toward the National Data Distribution Center. In a parallel effort, Don Vredeveld and Bob Reid (not MCC members) have sparked interest in a data base for use in ChE design calculations.

Activities now emerging are participation in standardization efforts, formulation of guidelines for effective computer program management, and involvement in AIChE government interaction and publicity efforts.

MINI/MICRO COMPUTERS: STATUS AND FUTURE

D. C. Haeske

Introduction

The applications of computerized systems are proliferating throughout industry and society, (1),(10),(11) and the chemical industry is in the forefront of development of these applications. From automated process design, dedicated and comprehensive process control, and molecular chemical analysis and synthesis to automated accounting, marketing and operations research, and financial modelling and planning, the chemical and allied industries are utilizing the powers of the computer to a greater and greater extent as time progresses. Additionally, as these applications grow and technology becomes more sophisticated, the applications themselves become more sophisticated. The early techniques of straight computation and batch processing have gradually shifted to more human-oriented information handling and network processing, frequently at great distance from the main computer center. Also, the physical size and cost per memory unit of main, high-speed computer memories have decreased so must that specific applications can be implemented in separate, dedicated data processors where cost effectiveness is more readily proven. Simultaneously with this memory size and cost reduction has come the ability to incorporate more and more preprogrammed functions into the relatively recently-developed read-only memories. This ability has enabled the inter-connection of many dedicated processors with one another, with existing large computers, and with many types of peripheral devices, such as 'intelligent' teletype terminals, television (CRT) displays, direct data-input media, and hierarchical storage devices. These provide organizations with their necessary inter-coordination through data summarization, consolidation, and long-range transmission.

The technology which led to the above reduction in memory size and cost as well as to the semi-permanent storage of preprogrammed functions was originally called minicomputing. This was traditionally defined as those computer processors with 8 to 16 bet word lengths having high-speed memories in the range of 4K to 16K words and which could be purchased for less than $10,000. The processors and memories of these minicomputers were initially oriented around the transistor but LSI MOS (large-scale integrated, magnetic oxide silicon) circuitry emerged, more functions were put onto a single chip, and production yields were increased in the semiconductor manufacturing processes. These led to the incorporation of the more frequently-used functions, such as the floating-point processor and integer multiply-divide, as well as such arithmetic functions as powering and functional transformation into the ROMs (read-only memories). This ROM function incorporation was the beginning of the technology now called microcomputing. (1),(2),(3),(9)

A feeling for the extent to which the mini-micro computer industry is progressing can be realized by a quote from Walter L. Anderson, currently associate director for ADP in the General Accounting Office. In a luncheon address delivered at a conference on minicomputers presented in San Francisco by the American Institute of Industrial Engineers in March, he said that the federal government "counted 90,000 minis in use throughout the world at the end of '73. They figure an additional 50,000 were installed in 1974 and more than that again in '75. By 1978 minis will account for 60% of the number of computers installed. The number installed in the federal government rose from 3,700 in '67 to 8,600 in '75. Further, he pointed out that "about one-quarter of the computers in 1967 had a cost under $50,000, whereas more than half the computers in 1975 had a cost under $50,000." (11) Thus, not only are minicomputers being installed at a high rate, but they also are adding greatly to the cost effectiveness of computing.

In order to provide a better understanding of this field, I will discuss in more detail where and how mini/micro computers are used, what different types there are, and what some of the problems are in their implementation. Finally, there will be a brief discussion of the projected future of the field as seen by some of its experts.

Major Applications (Where and How Mini/Micro's are Used)

The two major areas where minicomputers have been used are the business (accounting, order entry and processing, marketing evaluation, and financial analysis and planning) and the so-called non-business (process control, scientific experimentation, inventory control, and applications previously under the province of custom-designed systems). In the former, "the minicomputer made possible small scale business processors, extending computerization to organizations which previously were restricted to: (1) the sharing of time on a large computer; (2) the processing of their data by a service bureau which possessed a large computer; or (3) manual and semi-manual methods. Small scale business computers ultimately ranged from the level of electronic accounting machines, up to systems which were more powerful, and in many cases also more expensive, than the 1401 and the 315 of the earlier generation." (1) The reason for the expensiveness of some of these systems was not in the cost of the minicomputer itself, but in the cost of such peripheral devices as a moving-head disk, a paper tape reader/punch, and a high-speed printer. As pointed out in reference 2, these three peripheral devices in 1972 accounted for about 75% of the total hardware cost of a typical minicomputer installation. The software development cost of these systems is frequently not mentioned but can be several times the hardware cost.

In the non-business area, minicomputers were used to "control scientific experiments, to upgrade the intelligence and control the operation of a wide variety of instruments and data collection operations, for the control of manufacturing processed, the allocation of inventory, and for the control of word processing systems", (1) as well as for custom-designed applications. In this as in the business area, a large majority of the hardware cost of the minicomputer system was in the peripheral devices attached to the minicomputer. As an example of this: in a minicomputer system for physical chemistry instrument automation which we installed and implemented in our corporation's Glidden-Durkee research laboratory, approximately 80% of total system hardware and supplied-software cost resided in the non-minicomputer parts of the system. The major non-minicomputer classes were: a dual-disk drive, digital and analog signal processors, console and remote teletypes, a dual cassette drive, and computer interfaces for the preceding and for an incremental plotter. Although these items were additional to the minicomputer, they were necessary for such functions of the system as:

1. Real-time storage-retrieval of instrument signal data and retrieval of data reduction and operations-scheduling routines from disk storage

2. Real-time sampling, conversion, and channel interfacing of analog and digital signals from instruments and control buttons to ready lights

3. Real-time response to and interaction with human instrument operators at remote locations.

4. Interactive console control of the system and development of application software.

5. Back-up storage of programs and data. (4)

It is evident that any application will require considerably more in the way of hardware than just the bare minicomputer. Real-time applications, of course, will need more devices and device-servicing units than non-real-time, but each application must be evaluated with regard to its own individual requirements. As time progresses, additional capabilities are being combined into single LSI units which cost less than lower-capability units previously did. These additional hardware items and capabilities can be classified in the same primary types used to classify mini and micro computers.

Primary Types

Minicomputers currently are categorized in terms of: (3)

1. Word Length: between 8 and 32 bits, with a preponderance in the 12 and 16 bit category

2. Memory range: 4K to 56K (but up to 1 million bytes is allowed)

3. Cycle speed: generally around 1 microsecond (but this has been decreasing to the hundreds of nanoseconds)

4. Number of registers: 1 to 32

5. Price: usually a basic price of under $20,000

6. Available peripheral interfaces and support software, such as disk drives, analog and digital I/O signal processors, operating systems, and program development support software.

Although the basic price is under $20,000, industry surveyors have included systems costing up to $250,000 in the category of minicomputers. This generally is because of the peripherals added to the basic system. As an application grows from straightforward computing to signal processing and real-time response to user requests, the hardware can grow from a computer having central processing, high-speed memory, disk storage, and a teletypewriter to one having analog and digital I/O processors and interfaces with multiple remote teletypes and interfaces. As devices are added, the I/O scheduling and control requirements become greater, and more sophisticated software is required. Applications tend to grow beyond their original limits, too, as users become more familiar with their systems and find they can do more sophisticated information processing. The main benefits of minicomputers in these applications is that they provide the capabilities of expansion and real-time computing with an initially low price and relatively small high-speed memory.

The qualities of low price and memory size are even more striking in the more recent field of microprocessors. Here, the ability to incorporate numerous processing and computing functions together in 'firmware' on one or a few interconnected boards at relatively low cost has expanded significantly the potential of providing large scale computing power to larger numbers of people in much more 'intelligent' applications. This ability came about through modularization and miniaturization: individual hardware functions - the CPU (central processing unit or micorprocessor), the ROM, the RAM (random-access memory), the I/O structure, and the clock - were separated from one another, their components were combined in LSI circuits, and each function was placed on a semiconductor chip. Although the chips are smaller in size by about two orders of magnitude and much less expensive than the minicomputer boards they replaced, they are at least as powerful and provide the user with the flexibility of interconnecting a few chips to build a variety of microcomputing systems. (7),(9) The differences between them and their minicomputer counterparts can be seen in a category table similar to the preceding one for minicomputers:

1. Word size: 4 to 8 bits, with words combined where necessary for data accuracy and memory addressability.

2. Memory range: 16 to 16K, with RAM's and PROM's (programmable read-only memories) being generally larger than the ROM's by at least a factor of four.

3. Cycle speed: generally at least 3 microseconds because of longer cycles necessary for equivalent operations.

4. Number of registers: generally the same as minicomputers, but dependent on the application; a tendency exists to combine functional units into a specific work length register (e.g., the IMP-16 sixteen bit register and arithmetic logic unit, RALU).

5. Price: from about $150 up.

6. Available options (such as amount of memory expansion possible, types of consoles available, and power supplies needed and provided), standard I/O interfaces, and software packages (such as assemblers, cross-assemblers, high-level language, and operating systems).

The preceding table of microcomputer characteristics does not show, however, how the micro- and minicomputer technologies differ nor how they are being combined in new applications. The functions of CPU, high-speed memory, and device interfacing which require as many as eight boards in a minicomputer are available now on one microcomputer board. The 4040 4-bit and 8080 8-bit microprocessors are equally as powerful as and more flexible than their minicomputer CPU counterparts. The ability to 'burn' or magnetically reprogram a set of operating and logic instructions into a ROM or PROM, respectively, can save a great amount of high-speed memory and speed up its accessibility. Finally, the modular character of the microcomputer hardware functions makes their use extremely attractive in limited applications such as cash register, automobile, and television automation, where the extensive minicomputer resources would result in overkill. However, the operating systems and software development packages available with microcomputers are not as extensive or as well-debugged as their minicomputer counterparts. The implementation of systems with them at present requires a high level of expertise in writing and debugging their hardware-oriented assembly language programs as well as in understanding and using the micro logic and circuitry. The field has not progressed to the point where the average engineer can apply the technology to his requirements without considerable study of it.

Minicomputers (as opposed to microcomputers) from their major manufacturers, Digital Equipment Corporation, Hewlett Packard, and Data General, have extensive software development packages, high processing speeds, and numerous other resources available to perform an overall application. This is changing rapidly as microcomputer manufacturers upgrade their equipment and absorb minicomputer expertise. However, minicomputer manufacturers are adding more microprocessing to their systems, with some like Data General manufacturing their own microprocessors.

Future of the Mini/Micro Computer Field

At the risk of making a self-defeating prophecy in this rapidly changing field, one can detect three major trends for the future:

1. More functions, both computational and control/operational, will be incorporated into micro 'firmware' and applications will become more 'intelligent'.

2. The number of dedicated applications will increase as more human information-processing chores (like automobile operation, home operation, and engineering design and evaluation) are automated.

3. More extensive computer-to-computer interaction and networking will occur, leading to greater integration of the computer into the communication media.

These trends make even more exciting the challenges which lie ahead in the development of computerized applications in business, the professions, and society in general. At this stage, it appears that the mini/micro computer field will be in the forefront of this development.

(References 5 through 8 have been included for the benefit of those wishing to do further reading in the field.)

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(8) Soucek, B., Minicomputers in Data Processing and Simulation, N. Y.: John Wiley & Sons, 1972.

(9) Teener, M. D., "Minicomputers and Microcomputers: Part 2 - Microcomputers, "Mini-Micro Systems, June 1976, pp. 44-57.

(10) Business Week Feature Report: "Minicomputers Challenge the Big Machines", Business Week; April 26, 1976, pp. 58-63.

(11) Yasaki, E. K., "The Mini: A Growing Alternative", Datamation, May 1976, pp. 139-142.

CALL FOR PAPERS

Two sessions on advances in chemical engineering computing will be held at the New York City meeting of the AIChE, Nov. 13-17, 1977. R. L. Motard is chairman, Irven Rinard is co-chairman.

Papers are invited that describe substantive contributions to the technology of computer applications:

1. New approaches or understandings in process modeling, both steady state and dynamic.

2. Operability studies in process analysis.

3. New program and data organizations for integrated process and project engineering.

4. Data banks and data base technology in engineering research.

5. New computer algorithms, languages and software developments.

6. Impact of new hardware technology such as graphics, mini- and micro-computers on chemical engineering problem solving.

Deadlines: Abstract (or full paper) and Proposal to Present form to chairman by March 1, 1977. Final manuscript to chairman by June 1, 1977. Address is Dept. of Chemical Engineering, Univ. of Houston, Houston, Texas 77004.

The second Trenton Computer Festival will be held April 30, and May 1, obviously at Trenton. It will cover all aspects of consumer and hobby applications of microcomputers and will include demonstrations. Thus it will be a mix of fun and interesting technology. Papers will be in one of two categories: formal @ 10 pages, and short @ 3 pages. Drafts and 75 word abstracts are required by Feb. 15. If interested, contact Dr. V. J. Tarassov, Western Electric Co., PO Box 900, Princeton, NJ 08540 or phone 609-639-2549. The general chairman of the conference is Dr. Allen Katz, Trenton State College, 609-771-2487. - by Alan Glueck

AUTOMATION IN AN INDUSTRIAL RESEARCH LABORATORY

W. E. Kaufman, F. J. Krambeck, C. D. Prater,
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Introduction

The Paulsboro Laboratory of the Mobil Oil Corporation is responsible for research, development and technical service for refinery processes and related products. Most of these processes involve catalysis and an extensive experimental program is required to support this effort. The bulk of this experimental program takes place in small laboratory reactors ranging from a few cc's of catalyst to a liter.

The key bottleneck in our process research and development activities has always been the rate at which experimental work could be performed and interpreted. To relieve this bottleneck approximately eight years ago an automation effort involving mini-computers was started.

From the beginning it was decided to use an in-house approach to insure that the system would efficiently meet our current needs and be flexible enough to accommodate the inevitable changes which occur in research programs. To develop the basic skills required, training courses were held for our chemists and engineers as an off-hours activity. From these initial training courses, a small group of people were chosen to design and develop the automation system. Since all of these people had previously worked with the pilot plants, they readily understood the needs of an effective automation system. We found it much easier to train our chemical engineers and chemists in computer technology than trying to teach petroleum technology to a computer scientist. By designing, building, and maintaining the system ourselves, we also avoided the frictions and hazards of poor communications inherent in depending on a third party. We very early recognized that a network of mini-computers would be easier to construct, maintain, and modify than a complex interacting system residing in a single large computer. The smaller elements in the mini-computer network enabled us to write simplified programs. It was also recognized that eventually a data management system would be required to handle the large amounts of data which the automation system would generate.

Data Acquisition and Control System

Figure 1 shows an overall view of the Paulsboro Laboratory data system. All pilot plants have an associated on-line chromatograph to provide detailed analysis of the products of reaction. A separate PDP-8 is used to control and obtain data from a number of pilot plants and another separate PDP-8 is used to control and record the output of the chromatographs. Eight pilot plants are generally connected to one PDP-8 while six chromatographs (detector) channels can be supported by another PDP-8. Typically 270 pure components or lumped components are identified by the chromatograph utilizing a multi-column system.

The computers are interfaced to the experimental equipment through digital-analog interfaces. They are typically mounted in an insulated and temperature-controlled enclosure. The on-consoles and display CRT's are also supported by these on-line PDP-8's to provide operators with current operatoring data and the ability to change control parameters.

Data Reduction System

Each of the on-line machines has a disc storage unit which is utilized both for program storage as well as data storage. When the data storage areas are approaching full capacity, this data is transmitted over high-speed lines to a system of data reduction computers. Again PDP-8's or PDP-11's were chosen for this system. In the system shown in Figure 1, one of the data reduction PDP-8's acts as a real time answering service and stores the data on a large disc which is shared by another PDP-8 operating in Fortran. This machine calculates material balances when sufficient data have been obtained on the disc.

When this system reached capacity, another PDP-8 added to provide additional material balance capability. Adding additional hardware was deemed easier than developing a more complicated time-sharing system in software. Another larger data reduction system involving coupled PDP-8's and PDP-11/40's has also been developed and is in use. The combination of the data acquisition and control system with the data reduction system gave a large increase in the number of experimental runs which can be made. For example, one set of pilot plants which had been utilized through the decade, 1960-1970, recorded a total of 2,000 completed material balances. These same pilot plants when brought into the automation system are now capable of performing 2,000 material balances in six months. This large increase in experimental data led to the need to develop an effective data base system to both store and retrieve this information.

APL Data Base System

In the original design of the data base system we had anticipated using a more or less conventional Fortran-based system. However, about six years ago we had begun using APL (A Programming Language) as a specialized language to solve linear algebra and linear differential equation problems resulting from chemical reaction kinetics. Through this use we recognized that the language had great potential for the storage, manipulation, and retrieval of large amounts of data. Briefly, this was true because the language treats vectors and matrices in an efficient manner and data bases are no more than sets of vectors and matrices.

The current APL data base system resides on IBM 370/168 located some 60 miles from Paulsboro at our Princeton Laboratories. Completed material balances from the data reduction system are sent directly via electronic links to the APL storage terminals located throughout the Paulsboro Laboratory. These terminals are connected to the 168 by means of high-speed telephone lines. Over half these terminals are of the graphical display type and are used to plot the data in a wide variety of graphical forms. The axis, grids, titles, and points are all automatically plotted with only a few simple APL commands. Least squares polynomial curves can be placed through the data with ease since their calculation represents only elementary operations in APL.

Most of our commercial processes have been represented by mathematical reaction kinetic models. Since many of these mathematical models also reside in the APL System, experimental data can be compared directly with the reaction kinetic predictions.

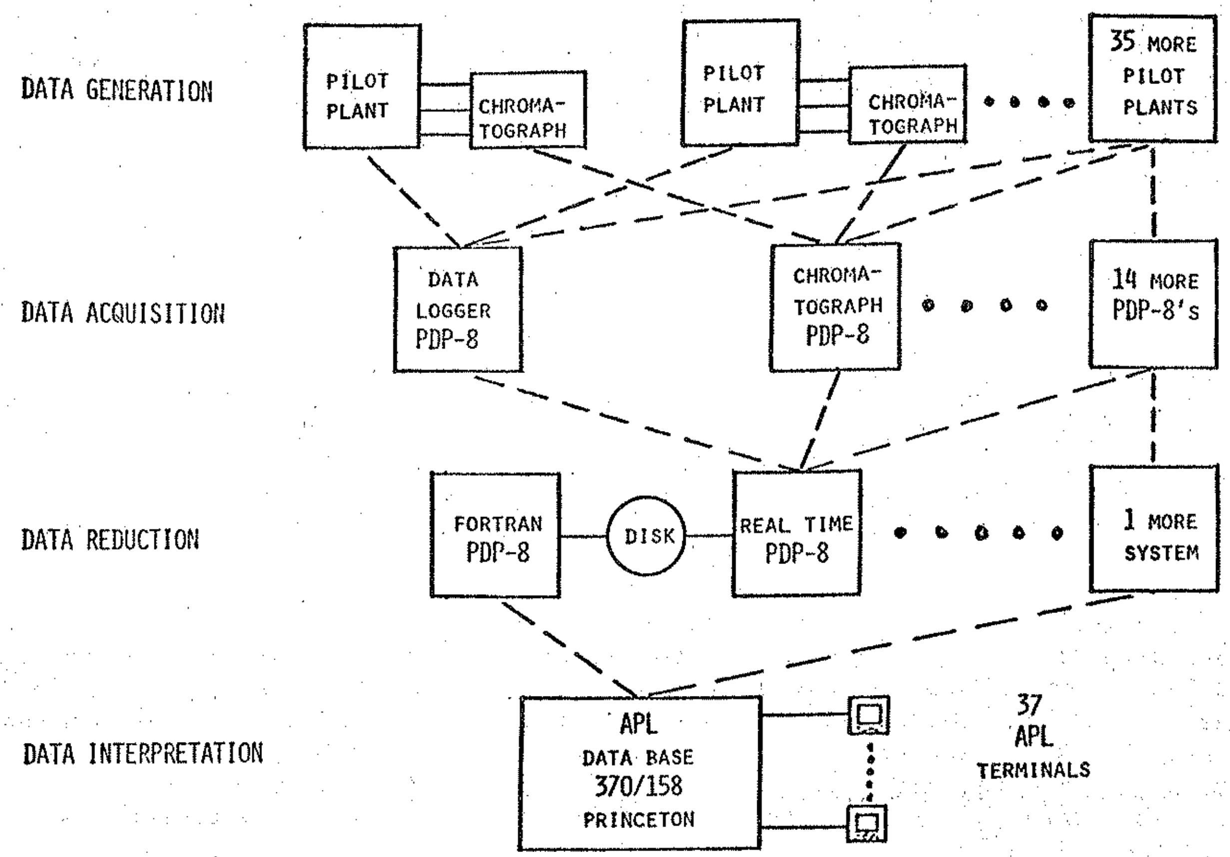
In addition to the automated pilot plant, experimental data from our analytical laboratories as well as our commercial plant data are also fed into the APL data base. In general, we have found the APL data system to be highly cost effective in storing and analyzing large amounts of laboratory as well as commercial data. Writing programs in APL has also proven to be highly efficient with an observed productivity gain of greater than five over performing similar programming in Fortran.

Summary

One of the key advantages of the overall laboratory automation system is the more effective focusing of our experimental program on our process research and development needs. Prior to the automation system sometimes four to six weeks were required before completed material balances were available. Only as this data slowly accumulated would it become apparent that a new direction in a research program was required. With the current system we can quickly spot important trends and adapt the experimental program to follow these leads almost immediately. The overall system has resulted in our ability to develop new processes and catalysts in a much shorter time scale than was previously possible.

FIGURE 1

PAULSBORO LAB DATA SYSTEM



SIAM (SOC. OF INDUSTRIAL & APPLIED MATH)
ACM (ASSOC. FOR COMPUTING MACHINERY)

Meetings of possible interest, including some non-SIAM and non-ACM are:

25-26 March 1977: ACM North Central Region Conference, Urbana, Ill. Program chmn: Alfred Weaver, Dept. of Computer Science, Univ. of Ill., 249 Digital Computer Lab, Urbana, Ill. 61801; 217-333-6755. (co-sponsored with Univ. of Ill.)

28-30 March 1977: Symposium on Mathematical Software, Univ. of Wisconsin; Contact C. W. de Boor, Mathematics Research Center, U. of W., Madison, Wis. 53706.

13-15 April 1977: ACM Symposium of High Speed Computer and Algorithm Organization, Urbana, Ill. Sponsors: NSF & Univ. of Ill. in coop. with ACM & IEEE-CS. Conference chmn: David Kuck, Dept. of Computer Science, Univ. of Ill., Urbana, Ill., 61801.

16-17 April 1977: AMS-SIAM Symposium on Computational Fluid Mechanics, at Biltmore Hotel, New York City. Contact AMS, PO Box 6248, Providence, RI 02940.

3-5 August 1977: ACM Conference on Management of Data, Toronto, Ontario, Canada. Sponsored with SIGMOD. Chmn: Frank King, IBM Research, Monterey & Cottle Roads, San Jose, Calif. 95193.

Publication: The ACM Transactions for September 1976 contains the following of interest:

"A Comparison of Algorithms for Solving Symmetric Indefinite Systems of Linear Equations" by Victor Barwell & Alan George.

"Hermite Interpolation using a Triangular Polynomial Basis" by Richard Bartels & Alec Steingart.

"Numerical Solution of Steady State Heat Flow Problems Over Curved Domains" by C. A. Hall, R. W. Luczak & A. G. Serdy.

"Algorithm 506.HQR3 and EXCHNG: Fortran Subroutines for Calculating and Ordering the Eigenvalues of a Real Upper Hessenberg Matrix" by G. W. Stewart.

EDITORIAL

It's almost a year since our first issue, this being our second. If this is a periodical, then we missed our period, and by the size of this newsletter, compared to the first, we are pregnant.

The editor, 10 Yorkshire Drive, East Windsor, NJ. 08520.

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CACHE

To clear the discrepancy in the May 1976 issue of CACHE News, the new officers are: Bob Weaver (of Tulane), president; Duncan Mellichamp (U. of Calif. @ Santa Barbara), vice-president; Rudy Motard (U. of Houston), secretary; and Larry Evans (MIT), executive officer.

An important objective is to make FLOWTRAN available. FLOWTRAN (developed by Monsanto) is on the United Computing Systems (UCS) network. In the school year 1974-75, 900 copies of the book, "FLOWTRAN Simulation - An Introduction" (by J. D. Seader, W. D. Seider and A. C. Pauls) were sold @ $10 to approximately 400 students and 500 engineers. 28 schools were involved. In 1975-76, 34 schools with 560 student users purchased 400 manuals. The average computer cost for using FLOWTRAN has been $40/student. In 1976-77 it is expected that 40 of the chemical engineering schools will be using FLOWTRAN. Professors who wish to use FLOWTRAN should contact the CACHE Corporation at the MIT office in Cambridge. They must sign a three-party agreement among themselves, the CACHE Corporation, and Monsanto Company agreeing not to use FLOWTRAN for private financial gain.

CACHE is in the middle of CHEMI (Chemical Engineering Modular Instruction), a NSF sponsored project to produce and distribute self-study, single concept, text modules in chemical engineering. About 400 total modules are involved in seven curriculum areas: control, transport, stagewise processes, design, material & energy balances, kinetics, and thermodynamics. The purpose of these modules is to augment a course where textbooks need supplementing. About 350 have already been commissioned. 150-200 are out for review. The present plan is to compile four modules within a single cover to sell for $1. Distribution and sales will be under the scope of Hal Abramson of the AIChE as part of Continuing Education. - Editor

PROJECT EVERGREEN

On Tuesday evening, November 30, 1976 a special event of the AIChE 69th Annual Meeting was held at the Palmer House in Chicago. The principal item on the Agenda was a presentation of Project Evergreen, a proposal of the National Bureau of Standards, Office of Standard Reference Data, by Dr. Howard White of NBS. Some 48 persons participated in the subsequent discussion.

This project has grown out of a consultation among several companies, NBS and Bob Reid of MIT. The proposal envisions the preparation of a data bank of the pure component properties of 1000 ubiquitous chemicals. Funding for the project is estimated at $100,000 per year of which one half would be raised by subscription from interested companies ($2,500 - 5,000 each). An advisory committee would be formed to counsel with NBS on the selection of substances and their properties and on the format for the dissemination of the products of the activity. Sponsors would acquire the results at a reduced price and non-sponsors would pay accordingly.

Properties to be included are the thermophysical, thermodynamic and transport properties. The data would be coded as to reliability and source. Missing data would be generated by estimation methods and so indicated.

The general consensus of the meeting was highly favorable to the idea. Considerable emphasis was placed on the machine readability of the project output. Although the industrial importance of mixtures is recognized, the project would not tackle these in the initial phase. Cooperation with existing data measurement and dissemination centers was judged to be important, including CODATA, an international committee promoting the dissemination of many types of data. CODATA was represented at the meeting by Jack Westbrook of General Electric, Schenectady.

The Machine Computation Committee will survey those who attended the meeting and any others who have expressed interest in the project to determine the likelihood of their organization's support. Consultations are continuing. Yet to be resolved is the location of the center and the organization of an umbrella organization. For a copy of the proposal, or to express your view, call or write to the Chairman of MCC's ad hoc Committee on this project: Dr. R. L. Motard, Dept. of Chemical Engineering, Univ. of Houston, Houston, Texas 77004, (713-749-2415). by R. L. Motard

ASTM COMMITTEE E-31 ON COMPUTERIZED LAB SYSTEMS

During 1976 this committee developed standard guidelines for specifying, implementing, evaluating and documenting computerized laboratory systems. In addition, E-31 is developing guidelines for specifying turn-key systems. These guidelines will provide the lab worker with a check list that should be considered when buying a fully computerized, vendor supplied lab instrument such as an emission spectrograph, etc. E-31 is working with Committee E-11 on Statistics to develop a versatile, user-oriented statistical package for handling interlab test data. At present, the NBS OMNITAB computer program is being considered for possible implementation.

In March, 1977, E-31 will conduct a symposium in Cleveland, Ohio on "Implementation of Computerized Laboratory Systems". Dr. George Barton and Jack Frazer, both of Lawrence Livermore Lab, are co-chairmen.

A new subcommittee, on Computerized Clinical Lab Systems, has been formed. Robert Megargle of the chemistry department, Cleveland State University, is chairman. He will preside over a symposium on automation problems in the clinical lab, to be held in Cleveland during March, 1978. - Editor

COMPUTERS & CHEMICAL ENGINEERING

Dick Hughes, editor of this new international journal, has sent proofs of the first issue to authors. Four papers have been submitted for the second issue; about 8 more are needed. This journal is intended primarily as a record of new developments in the application of computers to chemical engineering problems. Major areas of interest include: process synthesis, analysis and design; dynamic analysis and control of chemical processes; design methods for chemical engineering equipment, including chemical reactors, distillation columns, extractors, etc; and applications of computing and numerical analysis in chemical engineering science. If interested, contact Dr. Richard R. Hughes, 1500 Johnson Drive, Madison, Wis., 53706.

BITS ON GAZING AT THE CRYSTAL BALL

A second list has been sent to heads of Computer Science departments or their equivalent. The questionnaire is expected to appear in its totality in the proceedings for the Denver meetings August 28-31, 1977. Round Two will summarize the results of the questionnaire. Round Three is the discussion at the Denver meeting where the predictions will be reviewed by a panel of experts.

BITS & PIECES (BYTES & PICOS)

The computer celebrated its 25th anniversary in 1976. In 1951, Remington Rand's UNIVAC I was installed at the Census Bureau, the first working computer. It had a 1,000 word memory and could make 1,900 calculations per second. Compare this to today's million word memories and ability to make about three million calculations per second.

Called or not called, God is there. - Carl Jung

Maturity is when you do what you should be doing instead of what you want to do.

Sainthood is when what you should be doing becomes what you want to do.

IF YOU DIDN'T RESPOND TO THIS FORM EARLIER, PLEASE DO SO NOW!

Division Status Evaluation

A group of AIChE members is considering the formation of an Institute Division which would represent interests in the area of the application of computers, mathematics, management sciences and control systems to chemical engineering. Since you have at one time or another expressed a professional interest in these areas would you please indicate your level of interest in such a Division in answers to the following questions.

1. Are you now a member of AIChE? Yes ( ) No ( )

2. Which one of the following statements best expresses your feelings about the formation of this division.

   ( ) I strongly support the formation of this Division and would join it, become active in its work.

   ( ) I support the formation of this Division and would join it.

   ( ) I think the formation of this Division is a good idea and would probably join it.

   ( ) I have no strong feelings about the formation of this Division and would wait and see if it was of interest to me.

   ( ) I doubt that this Division should be formed.

   ( ) I don't think this Division should be formed and I would not join it if it was.

   ( ) I object to the formation of this Division and will work against its formation.

3. If the Division is formed, what areas of applications or disciplines should be specifically involved on its scope of activities (check more than one if appropriate).

   ( ) Computer Applications
   ( ) Mathematical Applications
   ( ) Applied Mathematics
   ( ) Process Control
   ( ) Process Synthesis
   ( ) Management Sciences
   ( ) Process Design
   ( ) Systems Analysis
   ( ) Others (please list)

   ____

   ____

   ____

4. If you would like to be on our initial organization mailing list, please note your name and address below:

____

____

____

Please send to attn:

Herb Owens
Asst. Secretary AIChE
345 E. 47th Street
New York, N.Y.10017

Thanks for your help!

Machine Computation Committee

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