ELECTION RESULTS
Vern Sterba

The results of the election held late in 1979 for 1980 officers are summarized below. Of 661 ballots mailed, a total of 306 were CAST (Sorry... but our newsletter editor loves puns). This is an excellent "turnout" and reflects the great interest of our members in the Division.

All Bylaw changes carried by a wide margin. The changes revised the newsletter publication interval from four to three times per year, extended the term of the Secretary/Treasurer to two years (and elected in even years), and established CAST's annual awards program. A complete, revised copy of the Bylaws can be obtained by sending a stamped (2 oz.), self-addressed envelope to the Secretary/Treasurer.

The term for officers is one year except for the Secretary/Treasurer who serves for two years (starting with the 1980 election). CAST Directors serve for three years. The Bylaws also assign certain responsibilities to selected officers as shown parenthetically. 1980 CAST Division Officers, Directors, and Committee Chairmen are listed below:

Chairman
Richard R. Hughes
Engineering Expt. Station
University of Wisconsin
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Madison, WI 53706
(608)263-1602

1st Vice Chairman
Bruce Carnahan
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University of Michigan
Ann Arbor, MI 48109
(313)764-3366

2nd Vice Chairman (and Awards Committee)
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Cambridge, MA 02139
(617)253-5461

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I.B.M. Corp.
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Michael T. Tayyabkhan (1980)
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P.O. Box 1026
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Thomas Edgar (1982)  
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Robert Harris (1982)  
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Midland Building - 206CB  
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Past Chairman (and Nominating Committee Chairman)  
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The CAST Newsletter is published three times per year by the Computing and Systems Technology Division of the American Institute of Chemical Engineers.
CAST programming sessions have traditionally been well attended, a fact which is most gratifying to our area chairmen. The continued high attendance by our membership is also helpful when we are attempting to schedule future meetings because CAST must compete with other divisions for a limited number of available sessions. A case in point is the Chicago meeting in November 1980. The National Programming Committee has received requests for more than 200 sessions in Chicago and can only accommodate 100. This is substantially less than the 130 sessions at the San Francisco meeting last November. This reduction is due in part to the meeting being shortened from four to three and one half days. Council decided in New York that the meetings would end at noon on Thursday. Attendance on Thursday afternoons has historically been poor due to members booking afternoon flights home.

In March Council considered inputs from members of Area 15c, notable Dale Seborg and has elected to continue AIChE's membership in the AACC. Because of this AIChE will continue to be one of the sponsoring societies for the Joint Automatic Control Conference.

Philadelphia Sessions


Population Balance Models in Chemical Engineering (1 session) Chairman: Prof. D. Ramkrishna, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907; Co-Chairman: H.M. Hulburt, Northwestern University, Evanston, IL 60201.

Portland Sessions

Use of Programmable Calculators in Chemical Engineering Education. Chairman: M.T. Tayyabkhan, Mobil Research & Development, P.O. Box 1026, Princeton, NJ 08540 (609) 737-3000 X2507; Co-Chairman: B. Krieger Dept. Chemical Engineering, Benson Hall BF10 University of Washington, Seattle, WA 98195.
Thursday AM: 15b Recent Developments in Control System Design and Estimation.
Chairman: Prof. G. Stephanopoulos, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455. Co-Chairman: E.H. Briston, The Foxboro Company, Foxboro, MA

**FOUNDATIONS OF COMPUTER-AIDED PROCESS DESIGN**

**July 6-11, 1980** - by Warren Seider


The program has been completed and copies are being mailed separately to all CAST Division Members. Persons interested in participating are invited to fill-out the Application Form accompanying the Conference Program and send it to:

Engineering Foundation
United Engineering Center
345 E. 47th Street
New York, NY 10017

The conference fee, which includes registration, meals, and accommodations (double occupancy) will be $360.

It is hoped that this conference, the first of its kind in the United States, will provide a forum for industrial practitioners having close contact with the problems to interact with researchers who are at the forefront of technical development. There will be eight formal sessions to the week-long conference, each covering important subfields. Each session will feature a "state-of-the-art" review followed by short presentations by active researchers, with ample time allowed for discussion.

Engineering Foundation Conferences were established in 1962 to provide an opportunity for exploration of problems and issues of concern to engineers from many disciplines. The format of the conferences is designed to encourage discussions on recent developments and to provoke suggestions concerning profitable methods of approach for making progress. It is intended that all attendees will participate actively in the discussions.

Attendance at conferences is by invitation or application. The conference fees, which include registration, meals, accommodations (double occupancy; single occupancy priced higher) and gratuities for the entire conference period will be announced latter.

**CALL FOR PAPERS - 1980 NPRA COMPUTER CONFERENCE** - by Vern Sterba

Some of you may not be familiar with the National Petroleum Refiners Association, but if you are a practitioner in the petroleum or petrochemical industry, your company is probably a member of NPRA. NPRA's Computer Conference is geared toward the practicing engineer and hence the papers generally concentrate on applications rather than theory. All attendees are provided with copies of all papers and the conference (and especially the question and answer session) has become a forum for the exchange of information relating to state-of-the-art techniques and equipment, who's doing what in computation and why, and where it's all going.

Papers are always well attended (no more than two concurrent sessions are ever scheduled so typical attendance would be 150-200) by engineers who attend this conference because they are interested in computation and the practical application of current computer technology.

Sessions currently planned for the November 16-19 Computer Conference in Philadelphia are:

- Distributed Process Control Applications
- Management Science Applications in Logistics
- Time Sharing Applications
- Energy Conservation - Computer Applications (panel discussion, Q & A Session)
- Environmental Health & Hazardous Substances
- Laboratory Systems in Automated Testing
If you have a potential paper for this conference, please immediately call the Program Chairman who will refer you to the proper Session Chairman:

Earl C. Gossett
ARCO, Harvey Tech. Center
400 East Sibley Blvd.
Harvey, IL 60426
(312) 333-3000

If you are interested in attending the Conference, additional details can be obtained from:

E. Lloyd Powers
Petrochemical Director
National Petroleum Refiners Assoc.
1899 L Street, N.W. Suite 1000
Washington, D.C. 20036

ASME - AUGUST 1980

The nuclear power industry response to TMI-2 includes a new major role for computers in performing a wide assortment of control and information processing tasks. Knowledgeable practitioners are concerned with the problems attendant to a massive, abrupt application of computer technology and recognize the need for broad-based understanding and discussion.

Currently, the situation is so dynamic that three special open sessions on this TMI subject have been arranged at the ASME 1980 International Computer technology conference being held in San Francisco on August 12-15, 1980. The conference keynote address is being presented by D.E. Haggerty, a commissioner on the president's commission for TMI-2 (Kemeny).

These open sessions will tie onto the three formal process control computer section presentations that include computer system development, Human Factor Engineering, and other related subjects. In this way the audience will include those able to provide candid, informed comments.

IFAC/81

8th Triennial World Congress, International Federation of Automatic Control, Kyoto, Japan, August 24-28, 1981. Theme: Control Science and Technology for the Progress of Society. Inquiries should be addressed to:

IFAC/81 Secretariat
Kinki Hatsumai Center
14 Kawahara-cho, Yoshida
Sakyo-ku, Kyoto 606
Japan

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A computer with as many vacuum tubes as a man has neurons in his head would require the Pentagon to house it, Niagara's power to run it, and Niagara's waters to cool it. WARREN S. MC CULLOCH, quoted in Robert Lindner's "Must You Conform?". (1956).

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Answers to puzzle on page 11.

1. A
2. C
3. A
4. B
5. C
6. A
7. B
8. B
9. C
10. C
Techniques for solving systems of nonlinear algebraic equations are featured in the books reviewed for this issue of the CAST newsletter. In so many areas of chemical engineering computing and simulation, at some point it often becomes necessary to solve a large set of nonlinear algebraic equations. In more cases than not, we all turn towards the Newton-Raphson method. The Newton-Raphson (N-R) method linearizes the functional equations which we wish to solve about our current guess of the solution and then solves for the root of the linearized equations to use as the next guess for the solution. Unfortunately, the N-R method is not perfect and some combination of poor initial guesses, highly nonlinear systems of equations, or numerical accuracy of our computer often leads to non-success. Indubitably, if we fancy ourselves as somewhat skilled in numerical analysis, we try and modify the N-R method so that we can find a solution to our system of nonlinear equations. If we succeed we often feel that we have developed a more rigorous technique until we try our "improvements" on another set of equations arising from a different simulation and find that our "improvements" were extremely model-dependent.

Alternatively, we turn to the literature or program libraries to which we might have access. With respect to the literature, three books which might serve as suitable references are:


The first book is actually a textbook while the second and third are conference proceedings. The textbook by Wait is a brief (158 pages) text divided into two essentially independent parts: Part I - Linear Algebra and Part II - Nonlinear Equations. Two-thirds of the text is concerned with nonlinear equations. Being a textbook there is an attempt at providing a thorough introduction to the theory of iterative methods which cannot be found in general introductory texts in numerical analysis. However, this text goes beyond the N-R method and gives practical methods that work in practical problems, together with some indication of the relevance of current theory to current practice. In addition there is an extensive bibliography that allows one to proceed to more detailed accounts of the various techniques and problems likely to be encountered in solving systems of nonlinear equations.

Wait has written an excellent guide to the solution of algebraic equations in a reasonable good format, with few typos, and unfortunately, insufficient examples.

The second and third books being conference proceedings are both more advanced and more specialized. Excellent chapters in both books have been contributed by C.G. Broyden. In the volume edited by Byrne and Hall, Broyden looks at quasi-Newton methods while in the volume edited by Rabinowitz, Broyden surveys the various developments in solving nonlinear algebraic systems. Both of these books contain computer programs for the solution of systems of nonlinear algebraic systems.

My preference of these two volumes, is that edited by Rabinowitz. I find that it covers the area of solving nonlinear algebraic equations more broadly than the volume by Byrne and Hall as well as being easier to read because it's typeset rather than reproduced from typed manuscript pages. However, your choice might be different based on your current interests. In order to help, since these books are not readily available at your local library, here are the chapter headings and contributors for each of these two volumes.

In "Numerical Solution of Systems of Nonlinear Algebraic Equations" edited by Byrne and Hall:

Nonlinear Algebraic Equations in Continuum Mechanics (W.F. Ames)
The Numerical Solution of Quasilinear Elliptic Equations (G.H. Myer)
Nonlinear Systems in Semi-Infinite Programming (S.A. Sustafson)
On the Solution of Large Systems of Linear Algebraic Equations with Sparse, Positive Definite Matrices (D.M. Young)

Some Computational Techniques for the Nonlinear Least Squares Problems (J.E. Dennis)

The Problem of Minimizing Nonlinear Functionals I. Least Squares (N.M. Steen and G.D. Byrne)

Quasi-Newton, or Modification Methods (C.G. Broyden)

Computer Oriented Algorithms for Solving Systems of Simultaneous Nonlinear Algebraic Equations (K.M. Brown)

On the Choice of Relaxation Parameters for Nonlinear Problems (S. Schechter)

The Contractor Theory of Solving Equations (M. Altman)

In "Numerical Methods for Nonlinear Algebraic Equations" edited by Rabinowitz:

A Review of Methods for Solving Nonlinear Algebraic Equations in One Variable (P. Jarratt)

The Determination of an Algorithm Which Uses the Mixed Strategy Technique for the Solution of Single Nonlinear Equations (P.F. Nedsore)

A Numerical Method for Locating the Zeros and Poles of A Meromorphic Function (L.F. Abd-ellal, L.M. Delves and J.K. Reid)

Recent Developments in Solving Nonlinear Algebraic Systems (C.G. Broyden)

Generalized Inverses for Nonlinear Equations and Optimization (R. Fletcher)

A Hybrid Method for Nonlinear Equations (M.J.D. Powell)

A Fortran Subroutine for Solving Systems of Nonlinear Algebraic Equations (M.J.D. Powell)

On the Convergence of Newton-like Methods (J.E. Dennis)

Matrix Iteration and Acceleration Processes in Finite Element Problems of Structural Mechanics (O.C. Zienkiewicz and B.M. Irons)

A Short Bibliography on Solution of Systems of Nonlinear Algebraic Equations (P. Rabinowitz)
MAXIMILL AN INTERFACE BETWEEN COMPUTER AIDED DRAFTING AND SIMULATION
Feature Article by Fred Thatcher

Background

Most modern chemical process flowsheeting systems utilize a high-level language to describe the process models needed, solution techniques and model connectivity. While these high level languages (CHESS, FLOWTRAN, ASPEN) have dramatically increased the useability of the simulation technology by providing an "engineer" oriented language, they stop short of highly automating his activities. The steps a design engineer follows in using a process simulator are:

1. Develop process idea.
2. Develop engineering flowsheet.
3. Develop computer process diagram.
4. Generate high-level language input syntax.
5. Simulate, analyze and debug.
6. Display results on flowsheet.
7. Compare cases, economic evaluation, parametrization.
8. Select process.

By taking a systems viewpoint of the engineering process, we need to ask, what set of automated tools will best enhance the overall engineering activity. Understanding the elements of this activity allows us to tailor a set of tools to assist the design engineer in all steps of the engineering cycle. We will attempt to demonstrate how these steps can be enhanced dramatically using combined computer aided simulation and computer aided drafting techniques. Furthermore, users may not just be highly technical, engineering design oriented individuals. They may be: Business Planners, Plant Engineers, R and D Planners, Plant Operators, and Policy Makers, who need to use simulation technology. By allowing this more general user to simply draw a picture of the process with only the assumptions and data required, then forcing the computer to construct the model block diagram, to develop the high level language calls, and to generate pictures, graphs and charts of the solution, we will allow a wider segment of the population to interact and communicate with the simulations and between themselves.

Our past experiences in utilizing graphics technology have been painful, in particular trying to generate a process diagram or computer diagram from a high level language syntax. Many available graphics packages are calls to FORTRAN libraries and require sophisticated programming knowledge to use. Constructing even modest engineering diagrams was an experience in trial and error. Hardware and communications were another bottleneck; in display CRT’s the resolution and image sizes were limited and the transmission speeds generally were limited to 300-1200 Baud.

Recent technical advances have totally changed the complexion of this environment. First, very sophisticated computer-aided drafting systems are available in the $75K-500K range and have experienced rapidly increasing use in industry. Examples of commercial drafting system vendors are Computer Vision, Applicon, Adage, M and S Computing...etc. These systems allow rapid generation of sophisticated process flow diagrams by moderately skilled technicians using a light pen, a menu of symbols and a graphical, shorthand, language-pattern recognition capability to communicate with these stand alone, minicomputer based systems. Since they operate at very high data rates (56K Baud), revisions to the diagrams are essentially instantaneous. The common use of these systems is to automate basic drafting operations like printed circuit masks, PID diagrams and construction diagrams. A skilled technician can produce a respectable plant diagram in 2-4 hours with no knowledge of software. Secondly, improvements in display hardware make general use
of graphics more attractive. Several fea­ures of note are 1. Higher resolution and 2. Logal storage-intelligence. Manufactur­ers like Tetronix, Hewlett-Packard, Digital Equipment and Megatek provide better per­formance in the $25K-60K range for an In­elligent graphic display processor. Final­ly, general graphics languages, which allow for rapid development of management displays are available and may be coupled with finan­cial analysis or simulation results. Ex­amples are DISSPLA, TELAGRAF, IGL, etc. The technical media are now available to link simulation and graphics technology.

THE MAXIMILL SYSTEM

The impetus for us to utilize graphics was much stronger than academic. One of our division vice-presidents requested a com­plete process simulator for our largest fiber complex. His first directive was that it be kept simple. There was an implied threat that if we built a simulation that re­quired an intimate knowledge of thermodynam­ics, he would find another consulting group. He compared our efforts with watching the Monday night football game: "When I watch the game, I really could...about elec­tronic circuit design." "Its your responsi­bility to make the simulator a useable tool" and he added, "put the complexity in the computer."

MAXIMILL -- we've put the complexity in the computer

We responded by building a highly graphics oriented optimization system based on the internally developed MAXIMILL modeling language. MAXIMILL is a joint development­al effort between Weyerhaeuser and Computer Sciences Corp. and is based on their software environment. The MAXIMILL system will now be discussed in technical detail to illustr­ate the techniques of graphics application.

The specific hardware used is:

1. Two APPLICON 880-PDPII-based drafting systems with six graphic display termin­als, digitizers, and two plotters. These systems reside in the central engineering facility.

2. TEKTRONIX 4014, 4016 intelligent graphic terminals with floppy disc drives, hard copy units, and 4662, 4663 plotters. These are used as medium cost devices for plant use.

3. Computer Science Corp. network primarily using UNIVAC 1108 and IBM 168 host sys­tems.

4. Internal HONEYWELL 6660 systems are used to collect plant process and financial data and to also generate MAXIMILL syntax. This is primarily a bulk data facility for data not entered from the graphics processor.

The specific software is:

1. APPLICON graphics system picture genera­tion software with shorthand symbol rec­ognition, macro facilities, a programm­able menu board, symbol recognition teach mode, component building mode in both a 2-D and 3-D environment.

2. The APPLE processor, a critical link which creates a machine independent ASCII file from the cryptically coded internal APPLICON format.

3. The LEW BARNESON processor which uses the APPLE file, separates the data from the graphics file and produces TEKTRONIX compatible output.

4. The MAXIMILL modeling language based on the SCIONIC mathematical programming system. MAXIMILL is a widely applicable process module library.

5. The GENERALIZED TEMPLATE LANGUAGE which allows specification of data, control, output and calculational elements to re­side on a graphic template.
6. The DISSPLA, TELAGRAF, and ENCORE graphics languages for bar charts, line graphs, etc.

7. The MANAGE and REPORT II generalized database and generalized report writing languages.

The MAXIMILL system, then, is a high-level graphical process flowsheet language which communicates with the user in the symbols he understands, and not in a pseudo process representation such as computer block diagrams and/or simulation symbols (GPSS, GASP) which require learning of another process representation dialect. Pictures generated on the APPLICON system are sent to the CSC computer, where they can be transformed into TEKTRONIX format. Since all of the picture generation occurs on the APPLICON system, it is not possible, currently, for a plant user to alter the structure of his picture. For our application, this is not necessarily bad, because it allows a quality check of the model by a central consulting staff before the picture and the model is altered. The plant users can pan and zoom over the pictures, change data and re-execute the simulation through a simple menu board dispatcher.

Remember to....

Keep it simple

Data from a plant process model may be required by a higher level region process flow model, or a subplant model may require data generated by a total complex model. To support this requirement, we allow direct interfaces between different pictures, or model databases. Therefore, as soon as several plants in a geographic region have optimized their individual facilities, the requirements for raw materials and marketing are linked to transportation and aggregate allocation models. For any process network in the system, there may be any number of users and any number of cases per user. Each simulation's results are aggregated to a total financial level and down to a sub-plant level. This allows templates to be created using summary as well as detailed process information. Reports and pictures may easily be composed from different networks, users, cases, levels. For example, a region picture could summarize the results of separate simulations from several different plants. Included in the general template language is the facility to perform calculations on system variables. This permits post-solution calculations to be inserted on any picture and even to be drawn from different networks, cases, users, or levels.

So far, we have used strictly 2-dimensional process representation in the pictures. However, we are now experimenting with 3-D process representation.

Purchasing graphics technology is a prickly affair, since there is a steep price/performance hardware curve. As minimum requirements for plant applications we have found: (1) local intelligence (2) local firmware for Pan, Zoom (3) resolutions of no less than 1K by 1K (4) 1200-2400 Baud minimum host to intelligent terminal speed (5) high level software support. It would be nice but it is not necessary to support full refresh graphics, color, 3-dimensional graphics, and local software.

RESULTS AND SUMMARY

Possibly the most gratifying element of the MAXIMILL modeling effort has been the enthusiastic reception of an understandable tool in the user community. We have been able to train a diverse cross section of the wood processing culture to construct and use optimization models, using this highly structured approach. The users range from highly qualified quantitative modeling experts to plant foremen with no previous systems or simulation experience. The practical rewards of doing this are very high, because it significantly expands our analytical staff capability. Further, the graphics format fosters better participation and commitment by management. It is simply easier to present a manager with a picture of his process and receive positive feedback, than if he gets a pile of computer listings. Finally, we believe that engineering modeling activities can be significantly more automated.
using closely coupled computer aided draft-
ing and computer aided simulation.

Biographical Note:

Fred Thatcher joined the Weyerhaeuser Com-
pany in 1969 as a programmer after complet-
ing a Bachelor's degree in Chemistry at
Eastern Washington State University. He is
currently a Senior Business Analyst in the
Fiber Systems Division and developed MAXIMILL
along with other software support packages.

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PUZZLE

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By checking up on the so-called truth in pro-
verbs, you also have a chance here to test
your own logical thinking: Decide quickly
(no more than five minutes is allowed for the
whole test) whether the two proverbs in each
group below A) express the same meaning, B)
contradict themselves, or C) have no relation
to each other whatever. Mark your answers
A, B, or C respectively, on a sheet of paper
and, later, compare them with ours. A score
of eight or over is very good.

1a) One swallow does not make a summer.
1b) One tree does not make a forest.
2a) Every cloud has a silver lining.
2b) Ambition has no rest.
3a) Shallow brooks are noisy.
3b) Little dogs bark the most.
4a) Out of sight - out of mind.
4b) Absence makes the heart grow fonder.
5a) Actions speak louder than words.
5b) The pen is mightier than the sword.
6a) A penny saved is a penny earned.
6b) A stitch in time saves nine.
7a) All things come to him who waits.
7b) The early bird catches the worm.
8a) Birds of a feather flock together.
8b) Two of a trade never agree.
9a) Necessity knows no law.
9b) Despair has often gained battles.
10a) Don't put all your eggs in one basket.
10b) Second thoughts are best.