



COMPUTING & SYSTEMS TECHNOLOGY DIVISION  
OF THE  
AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

NEWSLETTER

FALL-1978

MIAMI EXECUTIVE COMMITTEE MEETING

As has been the practice in the past, the CAST Executive Committee Meeting in Miami will be held on a Monday afternoon (November 13) from 1:30 to 5:00 pm. As usual, the meeting is open to all CAST members (in spite of the fact that someone at AIChE National Headquarters keeps ignoring our requests and putting an announcement--meaning it's for the executive committee only).

So if you want to become active in any of CAST's many committees, have some inputs or questions for the executive committee, are interested in how the committee works, or just want to meet the officers, by all means stop in. The rooms scheduled for this meeting are 208-209 in the Americana, but check the meeting list posted in the registration area Monday morning as last minute changes are sometimes necessary.

FIRST ANNUAL CAST DIVISION DINNER (GALA)

Join our colleagues in Miami for the first annual CAST Division Dinner. It will be held Monday, November 13, 1978, with a Dutch treat bar at 6:30 pm and dinner at 7:30 pm.

The featured speaker is Dr. Stuart W. Churchill, Patterson Professor, School of Chemical Engineering, University of Pennsylvania. Dr. Churchill plans to provoke our grey matter with his topic:

WHEN IS COMPUTING NECESSARY?

This dinner is listed as an AIChE event. Purchase tickets when you register. See

meeting program booklet for dinner location.

A PROFILE OF STUART CHURCHILL

Stu Churchill is the Carl V.S. Patterson professor of chemical engineering at the University of Pennsylvania. He has a fine record of technical accomplishments, service to the chemical engineering profession, and participation in AIChE activities.

His research, teaching and consultation have encompassed chemical kinetics, mass transfer and fluid mechanics, but has focused primarily on natural convection and combustion. His research and publications have been recognized by the Professional Progress Award in 1964 and the William H. Walker Award in 1969 of the AIChE. He was a director of the AIChE during 1961-67, vice-president in 1965 and president in 1966.

On top of this, Stu has boundless enthusiasm for living. He selected those wines we enjoyed at the University of Pennsylvania Museum last June. He keeps in shape by running regularly. His wife is charming.

If you ever heard him talk, you know that his presentations are never dry, never dull.

BALLOTING PROCEDURES

Election time is here. Article VI, Section 1 of the bylaws states that:

The Chairman, First Vice Chairman, Second Vice Chairman, Secretary-Treasurer and two Directors shall be elected annually by letter ballot sent to the members of the Division on or about October 1. Election shall be by a majority of those voting.

Tabulations of the votes shall be made by a Tellers Committee consisting of three Division members (not candidates for election nor members of the current Nominating Committee) duly appointed by the Division Chairman with the approval of the Executive Committee. Letter ballots shall include notice of the date by which they must be received in order to be counted, and that date shall be no earlier than four weeks after the mailing of the ballots. Ballots received after this date shall not be counted. The count shall be certified to the Executive Committee.

The ballots will be sent out by Bob Fisher, Secretary/Treasurer. Get your vote in.

#### CAST DIVISION PROGRAMMING

##### MIAMI

Computers in Process Design and Control (2 sessions)  
Impact of New Developments in Computer Hardware  
Impact of New Developments in Computer Software  
Free Forum in Programming Projects  
Recent Developments in Control and Estimation  
Education in Process Control

##### HOUSTON

Optimal Allocation in Energy Networks  
Simulation of Fossil Fuel Related Processes  
Sparse Matrix Computational Methods  
Microprocessor Technology in Process Control Applications  
Process Control Techniques  
Application of Improved Control Methods to Batch Processing  
Distillation Column Control Strategies  
Control Systems for Energy Management/Energy Conservation  
Computers in the Plant  
Computer Control: An Industrial Case History  
Compressor Control

##### BOSTON

Finite Element Methods  
Process Synthesis Methodology - A Critical Evaluation  
Computers in Education and Training

##### SAN FRANCISCO

Process Dynamics and Control  
Computers in Design and Control  
Applied Mathematics in Chemical Engineering  
Personal Computing  
Free Forum in Computer Technology  
Computing in Cost Estimating and Forecasting (2 sessions)  
Computing in Project Management (2 sessions)

Details of the charter for CAST division programming will be available at the Miami meeting, and hopefully will be published in the next newsletter.

#### AIChE AREA 15a (FORMERLY 1d) PROJECTED SESSIONS FOR 1978-79

Miami - November 1978

Computers in Design and Control  
W.D. Seider (University of Pennsylvania)  
L.C. McCune (Monsanto Co.)  
Impact of New Developments in Computer Hardware and Software  
R.S.H. Mah (Northwestern University)  
D. Prater (Mobil Research and Development Corporation)  
Free Forum on Computing Technology  
I. Rinard (Halcon Research and Development Corporation)  
R. Stanfield (Exxon Research and Engineering Company)  
Productivity in Programming Projects  
M.L. McGuire (Chemshare Co.)  
N.E. Rawson (IBM Corporation)

Houston - April 1979

Optimal Allocation in Energy Networks  
R. Pike (Louisiana State University)  
F. Pitts (Lamar University)  
Simulation of Fossil Fuel Related Processes  
L. Evans (Massachusetts Institute of Technology)

Simulation of Fossil (Con't)  
L. Joseph (University of Illinois  
at Chicago Circle)  
Sparse Matrix Computational Methods  
R.S.H. Mah (Northwestern University)  
A.W. Westerberg (Carnegie-Mellon  
University)

Boston - August 1979

Finite Element Methods  
B. Finlayson (University of  
Washington)  
S. Churchill (University  
of Pennsylvania)  
Process Synthesis Methodology -  
A Critical Evaluation  
D. Spriggs (Union Carbide)  
J. Siirola (Tennessee Eastman  
Company)  
Computers in Education and  
Training  
G. Marr (duPont)  
R. W. Southworth (William & Mary)

San Francisco - November 1979  
Computers in Design and Control  
J. Douglas (University of  
Massachusetts)  
E. Rosen (Monsanto Co.)  
Personal Computing  
M. Tayyabkhan (Mobil Research and  
Development)

Dale E. Seborg (U of Calif., Santa  
Barbara)

Houston AIChE Meeting - April, 1979

Sessions coordinated by Dale  
Seborg (ibid) and Cecil L. Smith  
(Louisiana State U)  
Since the abstracts were to be  
mailed to the session coordinators  
or the appropriate session chairmen  
by Sept. 15, it serves no useful  
purpose to give their addresses,  
because of the timing. There will  
be eight sessions on process control.  
Following are the session titles and  
chairmen:

1. Microprocessor Technology in  
Process Control Applications -  
Wayne Ralph (Proctor and Gamble)
2. Process Control Techniques  
(Jay Bailey, U. of Houston)
3. Application of Improved Control  
Methods to Bath Processing -  
David Fraade (Burroughs Wellcome)
4. Distillation Column Control  
Strategies (Thomas F. Edgar,  
U of Texas)
5. Control Systems for Energy  
Management/Energy Conservation  
(James W. Lane and Thomas Tsai  
Tenneco)
6. Computers in the Plant (Donald  
Griffin, Applied Automation)
7. Computer Control: An Indus-  
trial Case History (Eli  
Nisenfeld, Fisher Controls)
8. Compressor Control (Greg  
Martin, Shell Development)

1978 JACC - Denver, June 1979

#### AREA 15b ACTIVITIES

Miami AIChE Meeting - Nov. 1978

1. Recent Developments in Control  
and Estimation - (2 sessions)  
co-chaired by John Seinfeld  
(Caltech) and Manfred Marari  
(U of Wisconsin)
2. Education in Process Control  
co-chaired by W. Harman Ray  
(U of Wisconsin) and

AIChE is the host society for this  
conference. Chairman - T. F. Edgar  
Dept. of Chem. Eng., U of Texas,  
Austin, TX - 78712  
Deadline for submission is Nov. 1,  
1978. Authors should show intent  
by submitting a title and abstract  
to the review person by Oct. 1, 1978  
(probably past the time you received  
this). In addition, a copy of the  
title and abstract should be sent to  
Prof. Edgar. The review persons are:

AIAA - W. F. Powers (U of Mich)  
ASME - Doug Limbert (Arizona State  
U)  
ISA - Leo Durbin (Texas A&M  
SME - Dick Hohn (Cincinnati  
Milacron)  
AIChE- George Stephanopoulos  
(U of Minnesota)  
IEEE - Stephen Kahne (Case Western  
Reserve U)  
SIAM - M. W. Wonham (U of Toronto)  
TAPPI- Mike Mihalick (Taylor  
Instrument)

#### PRODUCTIVITY IN PROGRAMMING PROJECTS

A symposium on the above theme, sponsored by CAST, will be held at the Miami meeting on Thursday afternoon, November 16th. Norm Rawson of IBM is chairman. Mike McGuire of CHEMSHARE is co-chairman.

Software development has not kept pace with hardware advances, and now increased programmer productivity is needed to lower costs.

The following papers will be presented:

A Brief Tutorial on Software Engineering - C. T. Nute, Case Western Reserve

The Application Development Process - A. J. Albrecht, IBM

Programming Productivity in the ASPEN Project - P. W. Gallier and E. Ng, MIT

APL and Programming Productivity in Modeling Calculations, Data Acquisition and Data Processing  
J. A. Mann, Case Western Reserve

#### COMPUTERS IN PROCESS DESIGN and CONTROL

Two sessions on the above area of interest will be held at the Miami meeting in November. The first session will deal with the mathematics of process analysis and optimization. The second

will cover several important aspects of process design, including:

- a) dynamics of distillation columns, and
- b) process synthesis and computer graphics.

This will be followed by a short poster session to permit discussion with the authors.

#### BYLAWS - WANT A COPY?

The latest version of the CAST Division ByLaws (by Bob Morris) may be obtained by either:

1. writing to the Secretary/  
Treasurer, Robert J. Fisher,  
222 Alders Drive, Blue Rock  
Manor, Wilmington, Del 19803

and send a stamped, self-addressed envelope (~ 20 ounces, \$.28); or

2. picking up a copy at the  
Miami meeting in November.

## NEWSLETTER STAFF

Sigmund J. Lawrence - Publications Chairman  
Rodolphe L. Motard - Feature Editor  
Edward Gordon - Feature Editor  
Joseph F. Zemaitis, Jr. - Review Editor

will be top banana in 1979. Warren's address is: University of Pennsylvania, Dept. of Chemical and Biochemical Engineering, 376 Town Bldg., Philadelphia, PA 19104 or phone him at his office (215) 243-7953.

## EDITORIAL - MY SWAN SONG

For three years I have worked as editor of this Newsletter. The first two years were as part of the Machine Computations Committee, predecessor of the CAST Division.

At that time, Charlie Ware, Administrator of the MCC asked me if I would be willing to take on this task, on the assumption that a "retired" member of the AIChE would have plenty of time for it. He didn't know that, although I was "retired" from the General Electric Co., I was working full time for Catalytic, Inc., as a Process Engineer. I accepted anyway, feeling that it was one thing I could contribute to the cause.

Every issue deadline came up with some information still lacking, except this one, when I had so much info that I had to do some culling. Thus, even though the Division is but a year old, the Newsletter machinery seems to be well broken-in.

I want to thank the members of MCC and CAST who have helped make this Newsletter good enough to catalyze a comment from Sylvia Fourdrimer that it has set a new standard for Division Newsletters.

I also want to thank my employer, Catalytic, Inc., for supporting me in this effort, not only for expenses in attending meetings, but also for stenographic help.

Now it's your turn. The Division needs a new editor for the Newsletter. The fancy title is Publications Board Chairman. If you are interested, contact Warren Seider, who as 1st Vice-Chairman this year

APL: A COMPUTER LANGUAGE FOR ENGINEERS - FEATURE ARTICLE BY C. DWIGHT  
PRATER, MOBIL R & D

---

APL (A Programming Language) is a computer language particularly well suited to those engineers who have little inclination to learn traditional computer languages, but who need to use the computer for analysis and manipulation of engineering data. In contrast to other computer languages which were designed to fit the computer, APL originated as a concise and clean mathematical notation, particularly suited to understanding and design of computers. It was realized early that such a clean and concise notation would make a good programming language. APL was implemented in 1966 in IBM as a programming language only after a number of years of development and use as mathematical notation. Two recent examples of its use as a mathematical notation are: D. L. Orth, Calculus in a New Key, and K. E. Iverson, Algebra: an algorithmic treatment. This difference in origin from other programming language is responsible for many of the properties of APL. As a programming language, APL is more like the mathematical notation that the non-computer oriented engineer already knows, and therefore he usually finds it easy to learn and use.

APL has proved to be a very powerful computer language, but because of its nature and origin, it is difficult to develop a compiler for it. In its present implementation, the computer must interpret each line of the APL program. This is both an advantage and disadvantage. It is a disadvantage because APL programs often take somewhat more computer time than the corresponding programs in another language such as Fortran. Our experience at Mobil shows that this difference in run time is very much less for properly written APL programs than most people think. In fact, in many cases the APL actually ran faster, since the APL program, because of the ease with which it can be programmed, is often better constructed than the corresponding Fortran program. We have found that programs with running times as much as twice that of the corresponding Fortran are suspected as being poorly written APL programs and we reprogram them. It is sometimes thought that APL should not be used for programs that are to be run frequently. Our experience has shown this not to be true and we have a heavy use of APL in such programs.

An advantage that we have found for APL is that APL programs are much easier and cheaper to write and debug than programs in other languages. While the price of computer hardware is decreasing, the costs of software development and modification are becoming an ever-increasing fraction of the overall cost of the use of computer resources. Therefore the ease of writing and debugging APL programs has been an important factor in the increased use of APL. Our experience at Mobil has shown that APL programs can be developed in one-fifth to one-twentieth the time it takes for the same program in Fortran. In fact, if the program is needed in another language, such as Fortran, it is useful and cost-effective to develop and debug a program in APL and then convert to the other language.

The interpretive nature of APL makes its natural mode of operation an interactive one. An APL terminal provides a desk calculator mode of operation with all the power of a large computer at the engineer's finger tips. The non-computer oriented engineer frequently finds APL an easy programming language

to learn and use. In contrast the computer specialist often finds APL somewhat difficult to fit into his operations. The reason for this lies in the nature of APL. Because APL was not designed to fit traditional computer architecture, the computer specialist is required to change the way he thinks about and develops computer programs.

The conventional programming approach is to spend considerable effort in the design phase in an attempt to avoid costly redesign and reprogramming later. This goal is difficult to achieve because it is hard to visualize and predict the performance of a complex system in advance. Instead, the APL approach involves implementation of a prototype system and its use with real data at a very early stage. These systems can be thoroughly tested and evaluated by the end user during the development process to arrive at a design that truly meets the goals. This approach may require changes in the organizational structure of the typical computer software development group.

One surprising aspect of the growing use of APL is its effectiveness as a programming language for business applications. This is because APL is very effective for manipulating large data bases and for easily making the frequent program modifications that are required for many business applications.

One criticism of APL that one often hears is that an APL program is difficult to read and document. This view results from the fact that APL inherently requires a reorientation away from the traditional method of program documentation and reading. In fact, APL programs are easy to read and document if an appropriate approach is taken.

There will be a symposium on APL in Engineering on Thursday morning at the AIChE Miami Meeting, November 12 to 16, 1978. One of the speakers will be the originator of APL, Dr. K. E. Iverson of IBM. He will discuss the nature and origin of APL. Professor R. P. Andres of the Chemical Engineering Department of Princeton University will speak on the use of APL in Chemical Engineering Education. Professor A. J. Perlis, Head of the Computer Science Department of Yale University, will discuss the computer science aspects of APL and its relation to other programming languages. Dr. F. J. Krambeck, Manager of the Systems Research Group, Mobil Research and Development Corporation, will speak on APL in an industrial chemical engineering environment.

GAS PROCESSORS ASSOCIATION -  
TECHNICAL DATA

---

In this issue of the Newsletter Computer Programs offered by GPA for Process Design application are briefly described. The programs, available from GPA headquarters, Tulsa, Oklahoma, are reasonably priced and have wide use in the Process industries. The Programs currently available from GPA are:

1. The following K-value, enthalpy and entropy predictor programs: 1) GPA K\* & H MOD II, incorporating several thermodynamic models, 2) Peng-Robinson, 3) Mark V. All programs are applicable to mixture of hydrocarbons and common non-hydrocarbons. Specialized features such as two or three-phase calculations, hydrate and multicomponent critical state property predictions are available within one or more of the programs. GPA K\* & H Mod II can also be accessed through GE, United Computing and University Computing time-sharing systems.
2. GPA/NASA Chemical Equilibria program incorporates data directed toward synthetic gas and combustion calculations.
3. GPA Properties 75 calculates thermodynamic properties for a known phase. The calculation methods incorporated within the program were evolved from Rice University Properties III program which also originated from GPA research.
4. K-Data Program contains curve-fitted coefficients for K-value charts contained within the GPSA Engineering Data Book. By Steve Newman

AMERICAN PETROLEUM INSTITUTE -  
TECHNICAL DATA

---

Continuing with the general description of the API Technical Data Book provided in a previous Newsletter, the organization of the Data Book is as follows: Chapter 1, General Data; Chapter 2, Characterization; Chapter 3, ASTM-TBP-EFV; Chapter 4, Critical Properties; Chapter 5, Vapor Pressure; Chapter 6, Density; Chapter 7, Thermal Properties; Chapter

8, Vapor-Liquid Equilibrium; Chapter 9, Water-Hydrocarbon Equilibria; Chapter 10, Surface Tension; Chapter 11, Viscosity; Chapter 12, Thermal Conductivity; Chapter 13, Diffusivity; Chapter 14, Combustion.

At recent API Subcommittee on Technical Data (STD) meetings:

1. Maintenance and revision to Data Book by Penn State staff who have the responsibility of keeping the Data Book current by reviewing the literature and undertaking detailed evaluation work. Their most recent work included preparation of a revised chapter on vapor-liquid equilibria, and presentation of data and correlation studies in the following areas: hydrocarbon VLE, vapor pressure, thermal conductivity, and petroleum fraction characterization.
2. Current activities on preparing a metricated version of the Data Book, an ongoing task, were reported upon.
3. A review was presented of work done by Professor Wilson of BYU Thermochemical Center on collecting and correlating equilibrium data for designing sour-water strippers for pollution abatement.
4. A report was made on work being conducted at Texas A&M University on compiling thermodynamic properties of compounds present in heavy oils, lignite and coal. This effort is partially supported by API funds.
5. Liaison reports were given on activities of the (a) Gas Processors Association, (b) CODATA (Committee on Data for Science and Technology) and (c) the proposed cooperative industrial data project, AIChE Design Institute of Physical Properties Research (DIPPR).
6. New experimental data projects recommended for funding in 1978 included: (a) Vapor-liquid-equilibrium on water/non-hydrocarbon/hydrocarbon systems, and (b) Vapor-liquid-equilibrium on hydrogen/non-hydrocarbon/heavy hydrocarbon systems. By Steve Newman



## CALL FOR PAPERS

### "Computer Applications to ChE Process Design and Simulation"

Sponsored by I&EC Division of ACS at Washington, D.C. meeting, September 1979. If interested contact the session chairman as follows:

1. State of Art: R.G. Squires, Purdue University, W. Lafayette, Ind. 47907
2. Modelling and Simulation of Industrial Processes: G.E. Blau, 1707 Bldg., Dow Chemical, Midland, Michigan 48640
3. Computation Techniques in Design and Simulation: G.V. Reklaitis, Purdue University
4. Optimization and Control of Chemical Processes: D. Mellichamp and R. Rinker, University of California, Santa Barbara, Calif. 93106

### COAL CONVERSION PROCESS SIMULATION PROJECTS AT PURDUE AND LEHIGH UNIVS.

Two parallel DOE research projects have been operating since the spring of 1976 and continue thru 3Q1979. The dual goals are:

1. To develop steady state (Purdue) and dynamic (Lehigh) simulation programs suitable for coal conversion process modelling, for unrestricted distribution.
2. To apply these programs to study one or more coal conversion processes.

Progress has been significant, in completion of steady state design, implementation, testing and largely documented. This includes a process equipment simulation and information processing system, material and energy balances, physical properties estimation, equipment cost data bank, and a flowsheet graphics program.

More details on this project will be presented in the next Newsletter.

### AMERICAN PRODUCTION AND INVENTORY CONTROL SOCIETY (APICS)

APICS has established a special Process Industry task force to study the use of production and inventory management in

the Process Industries. They are adding Process Industry seminars to their meetings and are publishing a newsletter called "Work-In-Process". Most of this information is centered on computer implementations. Contact Richard Heard, Phillips Petroleum Co., Bartlesville, Oklahoma 74004 to get on the distribution list. (Telephone: 918-661-5419).

The next program will be held in Hollywood Florida, October 24-27, 1978 - Production and Inventory Management in the Process Industries - Workshop plus 10 papers. Richard Heard will chair. The intent of the program is:

1. To describe a variety of successful P&IC systems in process industries.
2. To review the state-of-the-art of P&IC applications in process industries, and
3. To describe the similarities and differences between piece goods and process P&IC principles and techniques.

At a recent seminar in Palm Springs, it was emphasized that successful inventory management in the process industries is based on established techniques and computer packages because they do work. The technique is to be considered satisfactory if it fits 80% of the cases. By Norm Rawson

### ACS - DIVISION OF COMPUTERS IN CHEMISTRY

The "National Resource for Computation in Chemistry" was funded 10/1/77 at the Lawrence Berkeley Laboratory. It will use the existing computer complex containing a DGD 7600, 6600, and 6400.

The NRCC is funded via a DOE/NSF grant for three years for a Phase I trial. The purpose is to obtain sufficient experience and justification for a Phase II proposal for a continuing and expanded facility.

The ACS Division of Computers in Chemistry will sponsor a symposium on Computer Assisted Drug Design for the Spring ACS meeting in Honolulu, April 1979. By Norm Rawson

UC COMPUTER GRAPHICS/MICROPROCESSOR  
DEMONSTRATION - AICHE ANNUAL MEETING,  
NOV. 12-16, 1978

The Computer Graphics and Real-Time Task Forces of the CACHE Corporation are sponsoring informal demonstration sessions on the use of microprocessors and computer graphics in chemical engineering.

The demonstrations are being coordinated with regular sessions sponsored by the new Division of Computing and Systems Technology, namely

- Impact of New Developments in Computer Hardware;
- Education in Process Control;
- Computers in Process Design and Control;
- Recent Developments in Control and Estimation.

Graphics equipment, microprocessors, and demonstration software provided by vendors and users will be made available to registrants at the Annual Meeting.

The facilities will be open on Tuesday and Wednesday afternoons (2:00 - 5:30 p.m.) and Wednesday and Thursday mornings (9:00 - 12 noon).

Persons wishing to demonstrate their own graphics or microprocessor software are encouraged to do so by making a demonstration tape or by operating on-line. Arrangements for on-line or tape operation should be made through Prof. Thomas F. Edgar, Department of Chemical Engineering, The University of Texas, Austin, TX 78712.

CODATA

CODATA is an interdisciplinary Committee of the International Council of Scientific Unions and is concerned with the compilation, critical evaluation, and storage and retrieval of data of importance to science and technology. The scope of CODATA includes primary quantitative data on the properties and behavior of matter and characteristics of biological and geological systems. The CODATA Secretariat is located at 51 Boulevard de Montmorency, 75016 Paris, France. Recent publications:

CODATA Bulletin

- No. 26 International Training Courses in the Handling of Experimental Data, 37 pp, January, 1978
- No. 27 Abstracts - 6th International CODATA Conference, 40 pp, March, 1978
- No. 28 CODATA Recommended Key Values for Thermodynamics 1977, 17 pp, April, 1978  
By Rudy Motard

BITS AND PIECES -(BYTES AND PICOS)

HELP! CAST division needs liaison representatives for AILE, AIP, AMA, APCA, ASC, ASIS, ASLE, ASM, ASOC, ASSE, SAI, SAMPE, TAPPI. If you are interested in such, or in helping Bob Lackmeyer in doing some liaison legwork, contact him at SOHIO, Midland Building, 427 CB, Cleveland OH 44115.

A free forum on computer technology will be held at the Miami meeting. This is for papers off the beaten track, to be presented in a less formal structure. Irv Renard of Halcon R&D (New York City) and Bob Stanfield of Exxon Res. & Engy. (Linden) are co-chairmen.

A symposium on sparse matrix methods in chemical engineering will be held at the Houston meeting (April 1979). Final manuscripts should reach the chairman, Dick Mah, at Northwestern University by Nov. 1.

Want to use any of this material in your newsletter? O.K. Just give proper credit.

---

SHIFTS-LEFT JUSTIFIED

R. L. Motard, Chairman  
Department of Chemical Eng.  
Washington University  
St. Louis, Missouri 63130

V.W. Weekman, Jr., Manager  
Catalysis Research Section  
Central Research Division Lab  
Mobil Oil Co.  
Princeton, NJ 08540

---

CANADA - SACDA AND ITS RESEARCH USE  
OF COMPUTING

The Systems Analysis, Control and Design Activity (SACDA) is an activity of the Faculty of Engineering Science at the University of Western Ontario. SACDA was started in 1973 under the Department of Industry Trade and Commerce program to set up Centers of Advanced Technology. SACDA works in the field of systems engineering with an emphasis on computer aided design and computer aided manufacturing (CAD/CAM).

SACDA is a high technology services activity with the resources to help industry through problem identification, model creation and problem analysis to achieve:

- A quick and economical reduction of practical and urgent engineering and economic problems to manageable proportions.
  
- A substantial savings in dollars and time by augmenting industry's own resources of people and facilities.

SACDA has proprietary programs for:

- Steady state and dynamic modelling and simulation;
- A growing library of system models;
- General problem solving;
- Rapid solution of large sets of linear and non-linear equations;
- Material properties packages and data files on ideal and non-ideal materials;
- Network partitioning;
- Manufacturing flow charts;
- Manufacturing scheduling.

By C. F. Shewchuk

## OFFLINE REVIEWS

By Joe Zemaitis, OLI Systems, Inc.

As a follow-up to the review of the various "popular computing" magazines, it should be mentioned that ROM has been merged into CREATIVE COMPUTING. In addition, BYTE has steadily improved and has become an excellent magazine for anyone interested in computing. The contents of BYTE should be of interest to most members of our division, since the articles are well written and cover hardware developments, software developments, an excellent language forum (which has made me take a serious look at PASCAL for some of our non-scientific projects), and features that generally run the gamut of interests of members of CAST.

Back to chemical engineering with some comments on the new journal Computers and Chemical Engineering. Finally, after several months of correspondence with Pergamon Press, I received the first volume of the journal and the first issue of the second volume. It appears that this journal will be an outstanding contribution to our field. The articles are most satisfactory, many coming from CAST members and some having been presented at AIChE meetings. Besides presenting new developments that lead to improved algorithms, some articles explore the use of flow-sheeting programs on developing process studies and modeling of new process concepts. This type of article is very worthwhile, since a presentation of strategies used by others is beneficial to all involved in process simulation. In addition, the review articles by Hlavacek on complex steady-state and transient behavior analysis and on process synthesis are quite rewarding.

There is one major fault - the cost of the journal is too high. Hopefully this is due only to start-up problems. Volume I cost \$64.00 and had only 203 editorial pages, for a cost of \$0.315 per page.

Volume II now costs \$71.00; hopefully it will have significantly more editorial pages. These high costs, when photocopying costs have dropped significantly, lead to a questioning of the "traditional" method of publishing technical papers.

An excellent new book was published this spring. Solution of Differential Equation Models by Polynomial Approximation by John Villadsen and Michael L. Michelsen. Prentice-Hall, Inc. (1978). This book attempts and succeeds at incorporating both model understanding and numerical analysis into a single volume.

After setting the stage in Chapter 1 by reviewing how mathematical models of rule processes are developed in chemical engineering, the authors point out how quickly complex differential equations arise which cannot be solved by the analytical techniques stressed in most undergraduate mathematics education.

This leads to a systematic treatment of the weighted residual techniques for both linear and non-linear systems of which the orthogonal collocation method is the authors' preferred choice.

In addition, a chapter is dedicated to one point collocation methods which are being explored and used with growing popularity since they provide a quick method of studying the influence of model parameters.

The text is well supplemented with necessary code listings and has annotated references at the end of each chapter (a device I most heartily endorse). Designed as a text suitable for either advanced undergraduates or graduate students, this book should aid those interested in modeling of chemical reactors or transport processes.