CAST AIChE

NEWSLETTER

COMPUTING AND SYSTEMS TECHNOLOGY DIVISION

American Institute of Chemical Engineers

VOLUME 3: NUMBER 2 NOVEMBER 1980

1980 CAST DIVISION AWARD

Paul Gallier

The winner of the 1980 CAST Division Award in Computing in Chemical Engineering is Professor Brice Carnahan of the University of Michigan. Professor Carnahan was recently chosen by the CAST Awards committee and CAST Director for his accomplishments both as a teacher and researcher in applications of computers. A founder of CACHE (Computer Aids for Chemical Engineering Education) and a past chairman of CACHE, he has been an inspiring leader in promoting the development and distribution of computer related educational aids among universities, industry and government. He has been the primary author of two widely used textbooks, "Applied Numerical Methods" and "Digital Computing and Numerical Methods". His books and short courses have served to teach a generation of non-computer experts how to make effective use of computing technology. He has directed development of the DYSCO computer program for generalized dynamic simulation of chemical processes and has written definitive papers on computer graphics. He is currently First Vice Chairman of the CAST Division.

The CAST Division's Computing in Chemical Engineering Award is given to recognize outstanding contributions in the application of computing and system technology to Chemical Engineering. The award consists of a certificate and $1000 and is supported by Chemshare Corp. and Simulation Sciences, Inc.

The award and plaque will be given to Professor Carnahan at the annual CAST dinner meeting at the Chicago meeting, November 19, 1980 at Burgoff's restaurant.

The CAST Awards committee consists of its Chairman Paul Gallier, the six Directors of the CAST Division, and five other AIChE members who are:

Professor James R. Fair, The University of Texas
Dr. Edward M. Rosen, Monsanto Company
Dr. Charles D. (Dwight) Prater, Mobil Oil Company
Professor Morton M. Denn, California Inst. of Technology
Professor Dale E. Seborg, University of California

CAST ANNUAL MEETING

The CAST Annual Meeting will be held Wednesday, November 19, 1980 at the Berghroff, 17 West Adams, Chicago, Illinois. A cash bar will be available at 6:00 PM and dinner at 7:00 PM. Reservations at $14.00 per person may be made via registration cards in your AIChE program book. The speaker for the evening will be Brice Carnahan, winner of the 1980 CAST Division Award. Dr. Carnahan's topic will be "Computers and Engineering Education - From There to Here to Where?"

EXECUTIVE COMMITTEE MEETING

The CAST Executive Committee will meet on Monday, November 17, 1980 at 11:00 AM. The room location will be posted at the meeting. Contrary to the meeting program, this will be an open meeting and all CAST members are invited to attend. A luncheon will be catered; those interested should contact Dick Hughes at (608)263-1602 for reservations.

IN MEMORIAM

We regret to announce that Ted Peterson died recently after a brief illness. Ted was a very active member of AIChE and the CAST Division. He was a division director at the time of his death. We are grateful for Ted's many contributions to our profession and extend our sincere sympathy to his family and friends.

PROGRAMMING - CHICAGO SESSIONS

Monday PM: 15a Thermodynamic Availability Analysis in Process Design and Synthesis. Chairman: Prof. Richard S.H. Mah, Dept. of Chemical Engineering, Northwestern University, Evanston, IL 60201. Co-Chairman: Prof. Richard A. Gaggioli, Marquette University, Milwaukee, WI 53233.

Monday PM: 15a Improvements in Finite-Difference Methods. Chairman: Prof. S.W. Churchill, Dept. of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 19104. Co-Chairman: Prof. J.O. Wilkes, Dept. of Chemical Engineering, University of Michigan, Ann Arbor, MI 48104.

Tuesday AM: 15a Computers in Process Design and Analysis. Chairman: Prof. A.W. Westerberg; Co-Chairman: Prof. I. Grossmann, Dept. of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213.

Tuesday PM: 15a Computers in Process Design and Analysis. Chairman: Prof. A.W. Westerberg; Co-Chairman: Prof. I. Grossmann, Dept. of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213.

Wednesday AM: 15b Microcomputer Process Control Applications. Chairman: Dr. J.D. Wright, Xerox Research Center of Canada, 2480 Dunwin Drive, Mississauga, Ontario L5L 1J9, Canada. Co-Chairman: Dr. P.A. Taylor, Dept. of Chemical Engineering, Mac Master University, Hamilton, Ontario L8C 4L7, Canada.

Wednesday PM: 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

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.

HOUSTON SESSIONS
April 5-9, 1981

15 Program Coordinator: Prof. Warren D. Seider, Chemical Engineering Dept., University of Pennsylvania, Philadelphia, PA 19104 (215)243-7953.

15a Modeling of Process Systems (1 session) Chairman-designate: Dr. H.V. Chien, The Monsanto Company, 800 N. Lindbergh, St. Louis, MO 63166.

15a Enhancement of Process Innovation and Development via Control Engineering (1 session, joint with area 15b). Chairman-designate: Dr. Irven Rinard, Halcon Computer Technologies 2 Park Ave. New York, NY 10016

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15a Optimization Theory and Applications (1 session). Chairman-designate: Prof. Ralph Pike, Chemical Engineering Dept., Louisiana State University, Baton Rouge, LA 70803.

15a Synthesis and Design of Plant Utility and Energy Recovery Systems (1 session). Chairman-designate: Prof. G.V. Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907; Vice-Chairman-designate: Mr. Donald E. Roush, Pullman-Kellogg, 3 Greenway Plaza East, Houston, TX 77046.

15b The Evolving Structure of Computer Control Systems for Industrial Processes (1 session). Chairman-designate: Dr. Mark Masek, Chevron Research Company, POB 1627, Richmond, CA 94807.

15b Distillation Controls in an Energy Conscious Environment (1 session). Chairman-designate: Mr. Ron Sorensen, Chevron Research Company, 576 Standard Avenue, Richmond, CA 94802.

15c Production Planning for Multi-Product Plants (1 session). Chairman-designate: Prof. G.V. Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907; Vice Chairman-designate: Dr. Michael Rinard, Merck & Co., Inc. POB 2000, Rahway, NJ 07065.

15c Project Control (1 session). Chairman-designate: Dr. T. Leininger, E.I. du Pont de Nemours Co., 3118 Louviers, Wilmington, DE 19898.

15c Computerized Cost Estimating (1 session) Chairman-designate: Dr. J. Woods, Pullman-Kellogg, 3 Greenway Plaza East, Houston, TX 77046; Vice Chairman-designate: Prof. G.V. Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907.

DETROIT SESSIONS (TENTATIVE) 1981

15a Chemical Engineering in the Manufacture of Computer Components (1 session). Chairman-designate: Dr. M.T. Tayyabkhan, Mobil Research and Development, P.O. Box 1026, Princeton, NJ 08540. Vice Chairman-designate: Dr. D.R. Mason, Dept. of Chemistry & Chemical Engineering, Florida Institute of Technology, Melbourne, FA 32901

15a Modeling of Coal Conversion Processes (2 sessions). Chairman-designate: Dr. Herbert I. Britt, ASPEN Project, Room 20-023, M.I.T., Cambridge, MA 02139. Vice Chairman-designate Christopher J. LaDelfe, TOSCO,Inc., Los Angeles, CA 90067. Co-sponsored with Area 11d.

15a Thermodynamic Availability Analysis in Process Design and Development. Chairman-designate: Prof. Richard A. Gaggioli, Dept. of Mechanical Engineering, Marquette University, Milwaukee, WI 53233. Vice Chairman-designate: Dr. S. Paul Singh, IGT, 3424 S. State, Chicago, IL 60616.

15c Engineering Productivity and the Computing Environment of the 1980's. (2 sessions) Chairman-designate: Dr. H.D. Spriggs, Union Carbide Corp., POB 8361, South Charleston, WV 25303. Vice Chairman-designate: B.F. Dickert, Union Carbide

NEW ORLEANS SESSIONS (PROPOSED) 1981

15 Program Coordinator: Prof. Richard S.H. Mah, Dept. of Chemical Engineering, Northwestern University, Evanston, IL 60201 (312) 729-0892.

15a Advances in Process Synthesis (1 session) Chairman-designate: Prof. Manfred Morari, Dept. of Chemical Engineering, University of Wisconsin, Madison, WI 53706.

15a New Approaches in Applied Mathematics (1 session). Chairman-designate: Prof. John H. Seinfeld, Chemical Engineering Dept., California Institute of Technology, Pasadena, CA 91125.

15a Computer-Aided Design of Batch and Semi-Continuous Processes (1 session). Chairman-designate: Prof. G.V. Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907.

15a Analysis of Nonideal Separation Systems (1 session, joint with Area 2c). Chairman-designate: Prof. Michael F. Doherty, University of Mass., Amherst, MA 01003.

15a Computers in Process Design and Analysis (2 sessions). Chairman-designate: Prof. Richard S.H. Mah, Dept. of Chemical Engineering, Northwestern University, Evanston, IL 60201

15b Control of Polymerization Reactors (1 session). Chairman-designate: Prof. Edward K. Reiff Jr., University of California, Berkeley, CA 94720.

15b Control of Catalytic Reactors (1 session) Chairman-designate: Prof. Edward K. Reiff Jr. Dept. of Chemical Engineering, University of California, Berkeley, CA 94720.

15b Restructuring of Undergraduate Education in Process Control (1 session). Chairman-designate: Prof. Manfred Morari, Dept. of Chemical Engineering, University of Wisconsin, Madison, WI 53706.

15c Scheduling of Process Operations (1 session). Chairman-designate: Dr. N. Rawson, IBM Corp., Dept. 83V, 10401 Fernwood Rd., Bethesda, MD 20034. Vice Chairman-designate: Prof. Richard R.S.H. Mah, Dept. of Chemical Engineering, Northwestern University, Evanston, IL 60201.

15c Graphics in Chemical Engineering (1 session). Chairman-designate: Dr. T. Leininger, E.I. duPont de Nemours Co., 3118 Louviers, Wilmington, DE 19898. Vice Chairman-designate: Dr. E.M. Rosen, the Monsanto Company, 800 N. Lindberg, St. Louis, MO 63166.

NOTE: All session chairmen for New Orleans should contact Dick Mah or Ralph Pike.

ENGINEERING FOUNDATION CONFERENCE ON CHEMICAL PROCESS CONTROL - January 19-23, 1981
The Cloister Hotel, Sea Island, Georgia

This conference will provide a unique opportunity for industrial practitioners and academic researchers to exchange ideas concerning new developments and the state of the art in chemical process control. The conference format is designed so that presentations by outstanding authorities will be discussed in depth by other authorities and all participants. Formal sessions are scheduled for the mornings and evenings; afternoons are left free for informal discussions. Since the conference attendees will eat their meals together in a separate dining room, there will be ample opportunity for them to become better acquainted and to exchange ideas informally. In order to permit adequate discussion in both the formal sessions and informally, the number of attendees will be limited to approximately 100. We anticipate having about 50 attendees from the industrial sector and 50 from universities.

The forthcoming conference is the second Engineering Foundation Conference on Chemical Process Control. The first conference, which was held in 1976 at the Asilomar Conference Site in California, was widely acclaimed to be very successful. The conference proceedings were published in the AIChE Symposium Series. (Foss, A.S. and M.M. Denn, editors, Chemical Process Control, AIChE Sympos. Ser., 72, No. 159 (1976).

Conference Organizers:

Dale E. Seborg
Dept. of Chemical & Nuclear Engineering
University of California
Santa Barbara, CA 93106

Thomas F. Edgar
Dept. of Chemical Engineering
University of Texas
Austin, TX 78712

Conference Sponsors:

The Engineering Foundation (New York City) and the Computing and Systems Technology Division of AIChE.

Preliminary Program:

Monday AM: Subject - System Software for Process Control. Chairman - M. Fjeld, Industrial Nucleonics (AccuRay).

Monday PM: Subject - Human Factors in Process Control. Chairman - M. Fjeld, Industrial Nucleonics (AccuRay).

Tuesday AM & PM: Subject - New Strategies for Process Control and Estimation. Chairman - W.H. Ray, University of Wisconsin.

Wednesday AM: Subject - Distillation Column Control. Chairman - T.F. Edgar, University of Texas.

Wednesday PM: Subject - Control Strategies for Energy Management and Energy Conversion Processes. Chairman - T.F. Edgar, Univsity of Texas.

Thursday AM: Subject - Design of Control Systems for Integrated Chemical Plants. Chairman - G. Stephanopoulos, University of Minnesota.

Thursday PM: Subject - Distributed Computer Process Control. Chairman - E.H. Bristol, Foxboro Company.

Friday AM: Summary - D.E. Seborg and T.F. Edgar.

CALL FOR PAPERS - 1981 JOINT AUTOMATIC CONTROL CONFERENCE - Charlottesville, Viriginia - June 17-19, 1981.

The 1981 Joint Automatic Control Conference (JACC) will be held in Charlottesville, Virginia during June 17-19, 1981. The conference program will include both contributed and invited sessions as well as tutorial and state of the art presentations in all aspects of the theory, application and implementation of automation and control systems. Topics of interest include, but are not limited to, linear and non-linear system theory, large scale system theory and decentralized control, estimation and identification. Presentation of control applications is strongly encouraged. Possible areas of application include, but are not limited to, aerospace systems, chemical process control, industrial and manufacturing systems, energy systems, biomedical systems, economic systems. Presentations concerning systems using microprocessor or computer implementations is also strongly encouraged. Papers relating to energy conservation, energy production and improved productivity will be especially timely.

Theme--Control Configured Design

Feedback control, frequently incorporating microprocessors, is increasingly an important initial consideration in the design of equipment. Control systems are no longer something to be added as an afterthought. The performance/cost relationships of aircraft, automotive equipment, production machinery, energy systems, appliances, testing equipment and many other items can be significantly improved by examining the potential contributions of powerful control systems and how the design may take maximum advantage of those contributions.

Some familiar applications--stability and performance augumentation of aircraft, active stress reduction systems for aircraft, automotive engine and transmission control for economy and pollution reduction, numerically controlled machine tools, industrial robots, direct computer control of production and testing, and HVAC systems control will certainly become more commonplace and new applications will emerge rapidly. Of special importance are active control systems for energy conservation and improvement of productivity.

The 1981 JACC will feature invited, contributed, tutorial and plenary sessions that emphasize the contributions of control systems to the design of better products and systems. The program committee particularly solicits authors and session organizers in this area.

Call for Contributed Papers

The 1981 JACC Program Committee is soliciting papers in all areas of control and automation. Two types of papers are solicited: (a) Regular papers describing work in some detail; (b) Short papers which present recent, perhaps preliminary results. All papers accepted for presentation will appear in the proceedings. However only regular papers will be considered by the author's Society for possible further publication unless the author states specifically otherwise.

Instructions to Authors:

Prospective authors should submit seven (7) copies of regular papers and seven (7) copies of a 700 word abstract for short papers marked "1981 JACC" by November 1, 1980 to the review person of the author's society. In addition, a copy of the title and abstract should be sent to Prof. Kenneth Knowles, Vice Chairman for Contributed Papers, U.S. Naval Academy Stop 14A, Annapolis, MD 21402, (301)267-3463.

Authors will be notified of the acceptance of their papers by February 1, 1981 and will be provided with a publication kit and instructions for preparing their manuscripts for the proceedings. Authors will be requested to limit their manuscripts to six proceedings pages or less. Short papers

will be limited to two proceedings pages. There is a page charge of $50.00 per page for longer papers.

Call for Invited Sessions:

The Program Committee is soliciting proposals for invited sessions in areas of interest for this conference. Prospective organizers should contact Prof. Gilmer Blankenship, Vice Chairman for Invited Sessions, Dept. of Electrical Engineering, University of Maryland, College Park, MD 20742, (301)454-6877 at the earliest possible date, but not later than November 1, 1980. They must also submit in writing by December 1, 1980 the session title, a 200 word summary, the list of papers with their titles, author's name(s) and address(es) as well as the names and addresses of the proposed session chairman and co-chairman. The proposed sessions will be reviewed by the Program Committee and final selection will be announced by February 1, 1981.

Short Calendar:

Deadline for Contributed Papers	11-01-80
Deadline for Invited Session Abstracts	12-01-80
Preliminary Selection of All Papers and Sessions	12-15-80
Final Program Established, Authors Notified	01-14-81
Author Kits Mailed, Programs Released	02-01-81
Deadline for All Preprint Material	04-03-81
Conference	06-17-18-81

1981 JACC Program Chairman:

Prof. Steve Dickerson
Mechanical Engineering
Georgia Institute of Technology
Atlanta, GA 30332

To shorten the delay please call (404)894-3255

Paper Review Chairman:

AIAA - Col. Allen D. Dayton
10221 Raider Lane
Fairfax, VA 22030
(202)692-0281

AIChE - Mr. Edgar H. Bristol
Research Department
The Foxboro Company
Neponset Avenue
Foxboro, MA 02035
(617)543-8750 ext. 2019

ASME - Dr. J. Lowen Shearer
Mechanical Engineering Building
Penn State University
University Park, PA 16802
(814)865-6377

IEEE - Prof. Michael K. Sain
Dept. of Electrical Engineering
University of Notre Dame
Notre Dame, IN 46556
(219)283-6538

ISA - Dr. Michael G. Rekoff, Jr.
School of Engineering
Univ. of Tennessee at Chattanooga
Chattanooga, TN
(615)755-4496

CHEMCOMP 1982 - CALL FOR PAPERS - CHEMICAL PROCESS ANALYSIS AND DESIGN USING COMPUTERS

May 25-27, 1982 - Crest Hotel, Antwerp, Belgium

15th European Symposium of the Working Party on Routine Calculations and the Use of Computer in the Chemical Engineering

Fields of Interest:

- Flowsheeting
- Physical and Thermodynamical Properties Data Bank
- Simulation of Polymer Processes
- Simulation of Coal Gasification and Liquefaction
- Simulation of Batch Processes

Deadlines for Authors:

05-01-81	Title and abstract (300 words)
05-15-81	Paper selection based
10-01-81	Complete manuscript for selection papers
10-15-81	Final paper selection
02-01-82	Camera ready copy

Symposium Committee:

Chairman: G. Froment, Rijksuniversiteit Gent, Belgium(*)

Members:
- H. Bussemaker, I.B.M., The Netherlands (*)
- J. De Leeuw Den Bouter, D.S.M., The Netherlands (*)
- B. Kalitventzeff, Universite de Liege, Belgium (*)
- J.-M. Kamp, Solvay, Belgium
- F. Theunissen, S.I.C.M., The Netherlands

Secretary: R. Viroux, Technologisch Instituut, K.VIV, Belgium

(*) Benelux members of the Working Party on Routine Calculations and the Use of Computer in the Chemical Engineering.

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Correspondence To Be Addressed To:

Symposium CHEMCOMP '82
c/o K.VIV
Jan Van Rijswijcklann 58
B-2000 Antwerp (Belgium)

COMPUTER-AIDED PROCESS DESIGN (CAPD) COMES OF AGE

Rapid advances in CAPD stimulated by process energy conservation and efficiency enhancement, new coal gasification and liquefaction processes, and the changing raw material situation have created an urgent need for industrial practitioners to interact with researchers and for experts to keep up with developments in other sub-fields. Such a forum was provided by the Engineering Foundation Conference on "Foundations of Computer Aided Process Design" which has just ended amidst enthusiastic acclaimations of its participants. It was the first one-week conference organized by the CAST (Computing and Systems Technology) Division of AIChE and also the first conference devoted to CAPD held in the U.S. 146 invited participants from 16 countries and 5 continents took part in the 8 technical sessions each featuring a state-of-the-art review and reports of latest advances in research and applications. The conference proceedings will be published in 2 volumes by the Engineering Foundation, and advertised and distributed by AIChE.

OFF LINE REVIEWS

Joseph Zemaitis, Jr.

In This issue two excellent books are briefly reviewed.

"Computer Calculations for Multicomponent Vapor-Liquid and Liquid-Liquid Equilibria", Prausnitz, Anderson, Grens, Eckert, Hsiek, and O'Connell, Prentice-Hall Inc., Englewood Cliffs, NJ (1980)

This is a completely new version of the monograph published in 1967 which is now out of date. The first section (142 pages) of this new monograph presents the basic theories for calculating both vapor-liquid and liquid-liquid equilibria. Topics covered include as per the chapter headings:

- Thermodynamics of Phase Equilibria
- The Vapor Phase
- The Liquid Phase
- Enthalpies
- Parameter Estimation
- Calculations of Equilibrium Separations in Multicomponent Systems
- Calculation of Vapor-Phase Nonidealities

The remainder of this monograph consists of several computer programs, test problems, and detailed documentation of the implementation of the techniques discussed earlier.

The chapter on the calculation of equilibrium separations is a concise, well written section which summarized various numerical approaches and points out possible pitfalls and experiences in solving phase equilibria. The discussion continues with a detailed description of the techniques used in their programs and why. In one short chapter, an entire subject is explored with extensive references and is indicative of the entire monograph. I highly recommend the acquisition of this volume.

"Separation Processes" 2nd ed., C. Judson King, McGraw-Hill Book Company, New York, NY (1980)

This book is a thorough revision of the first edition and should be useful to many not only for its thorough introduction to various separation processes, but also because of the care taken in this edition to consider the numerical computations of single or multistage separation problems. Though only computer code for one simple fractionation tower program is given, there are extensive discussions on the computations involved in computing multicomponent multistage separations as well as single stage separations. Considerable effort has been made to present and review the various algorithms used in the computations. In addition such topics as convergence problems and alternate techniques for initializing the iterative techniques are presented and evaluated.

In addition to the sections described above, this text discusses the many aspects important in the design of separation processes and should be a basic reference for those involved directly or indirectly in this area. The size of this text has grown from the first edition and the significant changes made in preparing this new edition are both worthwhile and welcome.

EDITORIAL * * * ARE WE ENGAGING IN ACADEMIC EXERCISES?

One of CAST's most important responsibilities is to provide a forum for its members to grow professionally and to share their experiences. We do this through our publications, meetings and programming. Those of us who seek this professional communion typically have one of three broad areas of interest: education, research and development and industrial applications. There is almost a flow of knowledge through these areas. The training and education of young engineers ultimately leads to the development of new systems technologies which finally come to fulfillment in industrial applications. The important aspect of this concept is that all three areas are essential to the continuing development of our profession. Without education there will be no new developments, without new developments there will be no new industrial applications, without new applications we can only look forward to stagnation.

What has CAST contributed in each of these areas? In education we provide meetings and programming and support CACHE. In research and development we provide publications, programming and special conferences. The bulk of our activities are in this area and we have been extremely successful. CAST sessions are among the best attended at National meetings and our conferences such as the recent Foundations of Computer Aided Process Design Conference are acclaimed.

CAST activities in the field of industrial applications have not been as outstanding. The early applications of computer based systems in industry had a reputation for overrun budgets, missed completion dates, overestimated returns on investment and poor reliability. While much progress has been made, our advancements here have not kept pace with our efforts in education and R & D. While we have provided for the feedforward of new technology, we have not provided an adequate environment for the feedback of practical experience.

The challenge facing CAST is to complete the circle of knowledge and experience; to provide programs, meetings and publications which benefit the practitioner as well as the educator and the researcher. If we are to call ourselves engineers we must accept and meet this challenge. If we choose to ignore it we must be content to merely engage in academic exercises.

Peter P. Hanik

PHYSICAL PROPERTY COMPUTATION TRADEOFFS

Alvin H. Larsen, Monsanto Company,
St. Louis, Missouri

Physical, thermodynamic, and transport properties provide a key foundation for chemical process design. One cannot hope to measure more than a tiny fraction of the physical properties needed for engineering design, and hence must predict, correlate, and compute them. Bringing the computer into the design picture means that physical property data must be made available to simulation and design programs on demand. Physical property models must then compute fast and with reasonable accuracy, be robust and reliable, give reasonable extrapolations, and make few if any demands on users. Several tradeoffs involving these factors and the engineering decisions in physical property computations become evident: computing speed vs. accuracy, specific vs. general models, decisions at user level vs. specialist level, flexibility vs. cost, and data evaluation vs. model development.

There is an increasing need for data in new ranges to satisfy energy conservation, pollution abatement, and competitive requirements. Greater demands are being made on the range, reliability, and variety of physical property models. Computers are being used more and more heavily for data evaluation and prediction. Computer tools such as interactive graphics and data base technology are making an impact on physical property computations. In such a rapidly changing environment, the tradeoffs have substantial economic importance.

Computing Speed vs. Accuracy:

Simple physical property models, such as linear or polynomial equations, compute quickly but may not be accurate enough, especially over wide temperature, pressure, or composition ranges. More complicated models may fit data within experimental accuracy or be thermodynamically rigorous but computationally prohibitive for simulation. As computing power increases and cost decreases, the tendency will be toward more rigorous and complicated models.

In process simulation recycle convergence (Evans et al., 1979) and flash calculations (Boston and Britt, 1978), the "two-tier" approach of alternately using simple and rigorous models appears very attractive. The complex models are used to generate the coefficients of the simple models which provide the iteration variables. The converged simple models then update the complex models, and the process is repeated until the change in the models from one update to the next is insignificant.

Physical property calculations are often at the lowest levels in the computing hierarchy and hence take a large fraction of simulation or design program computing time. To be most effective, the two-tier approach must therefore include physical property models. By careful program design, we can obtain the benefits of both computing speed and accuracy.

Specific vs. General Models:

Physical property models applicable only to a single component or class of components, phase, or limited range of operating conditions may be highly accurate and also compute quickly for specific cases. More general models may be inaccurate for some types of components or ranges, or may be much more complicated. Few if any models are completely general.

For example, special equations of state for a single component, such as water, are highly accurate but can be effectively used in simulation only when the increased accuracy from the special equation is more than worth the burden of including it along with general equations for other components. Cubic equations of state, such as Redlich-Kwong and its modifications, are quite general but may not be accurate enough near saturation or the critical point. Additional correlation constants for each component and for pair interactions improve the accuracy but limit the generality of the equation, since the additional constants won't always be available.

A closely related tradeoff is estimation vs. data correlation. To be useful, estimation methods must be general so they may be applied whenever data are not available. Even when data are available, an estimation may be acceptable or even preferred. Experimental data can usually be fit to some equation form, using enough specific

correlation constants. Extrapolation beyond the range of the data is then very risky.

An appropriate compromise here is to use whatever experimental data are available, if any, within the context of a generalized estimation method, to generate points over a wide range. These points are then fit by an empirical correlation, the coefficients of which are stored for later use. This approach has been found successful for liquid enthalpy data together with heat of vaporization and liquid heat capacity data (Larsen, 1977).

Decisions at User Level vs. Specialist Level:

Some companies choose to leave their process engineers responsible for the reliability of the data they use. Such engineers may not have the time or expertise to do data evaluation or model selection. They may use inadequate data or inappropriate models and be lured by an attractive computer printout into believing the results. Other companies have a group of physical property specialists responsible for locating, evaluating, organizing, and disseminating data and selecting or developing physical property models as required for engineering design. The specialists may not fully appreciate specific project data needs.

Of course, it is possible to have both user responsibility and specialist support. But then the engineers may not recognize when they need help, and the specialists may have difficulty selling their services without strong management support.

Flexibility vs. Cost:

If there are no options available, such as alternative models, the cost for computing properties may be low but the capability may not be adequate in many cases. Added flexibility results in more options and decisions, which extends the capability but increases the total cost. With ultimate flexibility, even the cost of understanding an enormous number of options and making intelligent choices becomes overwhelming.

An attractive compromise is to provide a small number of significant options, selected to satisfy predominant needs. Then the available capability will usually be adequate, but special problems will have to be treated separately.

Data Evaluation vs. Model Development:

Resources may emphasize systematic evaluation of available data or development of models to predict or correlate data. Actually both are necessary. Experimental data are limited so models must be available to predict missing values and compute values for simulation. Conversely, development of good models depends on evaluated data. Too often critical evaluation of data is slighted in model development. Shortcut design methods may be used effectively to estimate sensitivity of designs to thermodynamic properties and identify where property data should be verified or upgraded.

Our challenge in considering these tradeoffs is to use physical property resources in the most productive manner. Quantifying the tradeoffs would permit the benefits to be maximized. There is a need for greater selectivity in data evaluation and modeling for engineering design, including development of a methodology to focus data effort for the highest payoff.

References:

Boston, J.F.,and H.I. Britt, "A Radically Different Formulation and Solution of the Single-Stage Flash Problem," Computers and Chemical Engineering 2, 109-122 (1978).

Evans, L.B. et al., "ASPEN: An Advanced System for Process Engineering," paper presented at the 12th Symposium on Computer Applications in Chemical Engineering, Montreaux, Switzerland, April 8-11, 1979.

Larsen, A.H., "Computerized Liquid Enthalpy Correlation for Process Simulation," paper presented at AIChE St. Louis Section Symposium '77, March 29, 1977.

Biographical Sketch:

Al Larsen is Engineering Superintendent, Physical Properties and Process Simulation, in Monsanto's Corporate Engineering Department. He obtained a B.S.Ch.E. degree from the University of Utah and a Ph.D. degree in chemical engineering from California Institute of Technolgoy. Al has twelve years

of experience in physical properties and process simulation development, application, and consulting at Monsanto.

CASTing MY FATE TO THE WIND

I have genuinely enjoyed being Editor of the CAST Newsletter for the past two years. The responsibility of publishing three newsletters per year has been both challenging and rewarding. After this issue is completed I will be passing this responsibility on to an as yet unnamed successor whom I hope will enjoy it as much as I have.

Looking back I can point to both successes and failures. I feel that the content of the newsletter has been relevant to the needs and interests of our membership. I have tried to concentrate the information on activities in our profession. Among the shortcomings, I had hoped to make the Newsletter much more of a forum for our members to express their ideas on the directions that our division should be taking.

I have been very pleased with the quality of the features, reviews and news articles I have been able to include in the newsletter. This is due to the efforts of the editors on the newsletter staff, Rudy Motard, Joe Zemaitis, Ed Roche and Ed Gordon. The capabilities and dedication of these gentlemen is truly outstanding and I wish to publicly thank them. Additional thanks go to my employer, Northern Petrochemical Company for their support of my activities. A final thank you goes to Vern Sterba for getting me involved in CAST several years ago.

At this writing Dick Hughes is seeking candidates for Newsletter Editor. I encourage those of you who are interested to call Dick at (608)263-1602.

Pete Hanik

Murphy's Law? Of course, EVERYBODY knows that one. But how about the following gems which appeared in the Del-Chem Bulletin (May 1979)?

BASIC PRECEPTS OF SCIENCE
according to Del-Chem

Rabb's Theorem: If the experiment works, you must be using the wrong equipment.

Horner's Five Thumb Postulate: Experience varies directly with the amount of equipment ruined.

Gumperson's Law: The probability of a given event occurring is inversely proportional to its desirability.

The Futility Factor: No experiment is ever a complete failure; it can always serve as a bad example.

The Compensation Corollary: The experiment may be considered a success if no more than 50% of the observed data must be discarded to obtain a correspondence with theory.

Sturgeon's Revelation: 90% of EVERYTHING is crud.

Fourth Law of Thermodynamics: Everything takes longer and costs more.

The Ultimate Principle: When you are investigating the unknown...you do not know what you will find.