



NEWSLETTER

COMPUTING AND SYSTEMS TECHNOLOGY DIVISION

American Institute of Chemical Engineers

VOLUME 2: NUMBER 3

NOVEMBER 1979

RICHARD R. HUGHES NAMED FIRST RECIPIENT OF CAST
DIVISION "COMPUTING IN CHEMICAL ENGINEERING" AWARD

The CAST Division Awards Committee is proud to proclaim Prof. Richard R. Hughes of the University of Wisconsin as the first recipient of the division award for outstanding contributions to computing in chemical engineering. The \$1,000.00 award, made possible by contributions from ChemShare, Inc. of Houston, and Simulation Sciences, Inc. of Los Angeles, will be presented at the CAST Division Dinner at the San Francisco meeting on November 26. Prof. Hughes will be the speaker for this occasion and his topic will be: "The Engineer or Computer - Which is the Boss".

Prof. Hughes has a long and distinguished career in both industry and academia following receipt of B.S., M.S. and Sc.D. degrees in chemical engineering from MIT. Because of World War II, his education was interrupted by services as an officer in the U.S. Army Ordnance Department - two years in the Mediterranean, and two years as an instructor at West Point. In graduate school, his research with Dr. E. R. Gilliland concerned "Extractive and Azeotropic Distillation" and "The Mechanism of Mass Transfer Inside Drops".

On completion of the Sc.D. in 1949, Dr. Hughes joined Shell Development in San Francisco, later consolidated at Emeryville, California, as a research engineer in fluid mechanics and mass and heat transfer, with special emphasis on drops and bubbles, fluidization, cyclone separators, vacuum flashing, and de-entrainment. This work was followed by an assignment as a process engineer,

with a major effort in catalytic cracking process design, and a brief tour as a refinery plant technologist. On return to the laboratories in mid-1957, he quickly became involved with computer applications, first in unit operations, then in simulation, optimization, applied statistics, and operations research. In the late 50's, the group effort he supervised led to CHEOPS (Chemical Engineering Optimization System), a major step in making process optimization practicable. In 1962, he moved into research management as a department head spending four years in applied mathematics and two more years in chemical engineering.

After twenty years experience with Shell, Professor Hughes joined the University of Wisconsin in 1968. Most of his research at the University has been related to the use of computing in chemical engineering; recent studies concern practical, efficient methods of optimizing processes using modular simulation systems, and better ways of handling uncertainty in process optimization. However, some effort has been devoted to environmental modelling, and one present study concerns magnetic ore separation. This research has resulted in five Ph.D. degrees, and

*** MEETING NOTICE ***

The CAST Division will hold its annual meeting and awards dinner in San Francisco on November 26, 1979. See article inside for details.

seven M.S. degrees. In addition to his research and teaching activities at the University of Wisconsin, he serves as Associate Director of the Engineering Experiment Station and Coordinator of Computing Activities for the campus. His administrative duties include the coordinated planning and development of all computing on the campus, under the direction of the Chancellor and the Vice-Chancellors, and general assistance in the administration of the research activities of the College of Engineering, under the direction of the Dean and the Associate Dean. Hughes has also had special administrative tasks. From early 1973 to mid-1974, he served (full time) as Assistant Vice-Chancellor charged with facilities development and planning, with special concern for the new Center for Health Sciences, which was then being planned and is now finished and occupied. Since May 1979 he has been serving as a special Data Processing Coordinator for the entire State government.

Dr. Hughes has been a member of the American Institute of Chemical Engineers since 1945. He served as Director in 1969-71, and has been active on several national committees. In 1962, he was chairman of the Machine Computation Committee. Currently, he is Treasurer of the Environmental Division, 1st Vice-Chairman of the Computing and Systems Technology (CAST) Division, and Vice-Chairman of the Continuing Education Committee. He has been a frequent lecturer in the AIChE Continuing Education program. He is a charter member and officer of CACHE, and also belongs to ACM, ACS, AAAS, ASEE, ORSA, TIMS, Sigma Xi, and the Econometric Society, and is a licensed Professional Engineer in the State of Wisconsin.

With encouragement and support of the AIChE Machine Computation Committee, Prof. Hughes started up the new journal, Computers in Chemical Engineering, a Pergamon Press quarterly, and currently serves as the Editor.

Prof. Hughes married soon after his graduation. He and his wife, Elizabeth, have three daughters and five grandchildren. His major avocation is music.

He sings (mostly Lieder) has studied piano and music theory, and is active in chorus and solo work with the Madison Civic Chorus and Civic Opera. In California, he enjoyed mountain hiking, but this is less available in Wisconsin. He is now an enthusiastic golfer.

B. Carnahan
Chairman, CAST Division Awards Committee

FIRST ANNUAL CAST AWARDS DINNER - SAN FRANCISCO AIChE MEETING - MONDAY, NOVEMBER 26, 1979

The Executive Committee of CAST Division invites you to join us on the occasion of our first Awards Banquet. We hope that you will be present to honor Professor Richard R. Hughes, the first recipient of the Computing and Chemical Engineering Award and to learn more about the progress of our young Division, which in August exceeded 700 members. Professor Hughes will speak on the subject "Computer or Engineer - Which is the Boss?"

VOLUME 2: NUMBER 3 NOVEMBER 1979

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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.

The dinner will be at A. Sabella's Restaurant on Fisherman's Wharf, a cable car ride from Union Square. A cocktail hour, with cash bar, will begin at 6:30 p.m. Dinner at 7:30 p.m. will be their Deluxe Buffet at a cost of \$18.00 (including tax and tips).

Preregistration with the card provided in your national program is strongly recommended. Reservations for the dinner may also be made when registering for the AIChE Meeting but must be completed before the AIChE Registration Desk closes at 7:00 p.m. on Sunday evening, November 25.

A. Sabella's can accommodate 150 people, but attendance in San Francisco is expected to be high and it is recommended that you preregister to be sure of obtaining a ticket. Even if space is available, reservations will not be accepted past Sunday evening, except under extenuating circumstances.

W. D. Seider
September 14, 1979

CHAIRMAN'S MESSAGE

On this the occasion of my last Chairman's Message, I am reminded of our progress during the first two years of the CAST Division. Probably the leading indicator, our membership grew to 450 in 1978 and during the first half of 1979 expanded to over 700. We are well on our way toward establishing our position as one of the leading Divisions of AIChE.

For many of us, the exercise of establishing awards, accepting nominations, selecting an Awardee, and arranging for appropriate publicity is a new experience. As we focus upon our first Awards Banquet, I want to recognize the efforts of Dr. Mike Tayyabkhan, first Chairman of the Awards Committee. Mike and his committee worked to define the awards, obtain funding from ChemShare Corporation and Simulation Sciences, Inc., create the appropriate Bylaws, and solicit nominations. At mid-year, Prof. Brice Charnahan (Second Vice-Chairman) assumed the position of Chairman (as stated in the Bylaws) and has oversseen the selection of the first awardee, Professor

Richard R. Hughes.

We were sorry to learn that, subsequent to his retirement from DuPont Company in June, Dr. Fred C. Stults, Chairman of the CAST Programming Board, was unable to continue in this role. Fred submitted his resignation to the CAST Executive Committee prior to the Boston Meeting of AIChE. The Executive Committee wishes to express its appreciation to Fred for one and a half years of service as the first Chairman of the Programming Board. It was not easy to coordinate three programming areas, which had previously operated autonomously, and Fred deserves many thanks for lending his years of programming experience in the early work of CAST.

Fred will be succeeded as Chairman of the Programming Board by Professor Richard S. H. Mah, who has served as Chairman of Area 15a, Systems and Process Design, for the past two years. Professor James M. Douglas will assume the responsibilities as Chairman of Area 15a.

Extensive plans have been made for Technical Sessions at future AIChE meetings by Areas 15a and 15c, Computers in Management and Information Processing, but communications with Area 15b, Computers in Process Control, have lagged behind. One of Dick's challenges will be to find ways for more active coordination with our colleagues in Area 15b.

If you would like to participate in CAST activities, and your contributions are welcome, let me suggest that you contact people directly to discuss the possibilities. It would also help for you to obtain a copy of the CAST Divisions Bylaws from our Secretary/Treasurer, Dr. Robert E. Harris. It is a credit to Robert L. Morris, Director of CAST, and his Division Formation Committee, that the Bylaws they created have enabled the Executive Committee to function smoothly during the early years of CAST.

There are many others who deserve acknowledgment for bolstering the services we provide for CAST membership. Rather than acknowledge every contribution, some of which are very sub-

stantial, I will close, having focused upon the most significant achievements of the last three months.

I have enjoyed being Chairman and working with many of you during the past year. I look forward to continued participation on the Executive Committee as Past Chairman.

W. D. Seider
September 14, 1979

HIGHLIGHTS OF EXECUTIVE COMMITTEE MEETING AUGUST 20, 1979, BOSTON, MASSACHUSETTS

Warren Seider proposed an amendment to extend the secretary-treasurer's term of office to two years. The amendment will be submitted to the membership.

Mike Tayyabkhan proposed an amendment restructuring the awards committee. Brice Carnahan was appointed as awards committee chairman. It was agreed that the institutional award and the student award will be postponed until next year. The committee congratulated Mike for his contributions as chairman of the awards committee.

A Bylaw amendment was submitted by Pete Hanik. This amendment would change the publication date and number of newsletters to correspond with AIChE meetings.

The nominating committee plans to have all ballots mailed by September 28 and all ballots counted by November 1.

Bob Harris reported that membership is presently about 700.

Ted Peterson reported that C³ is working with National to review upgrading their IBM 370/40. A study also indicated that computerized registration at National meetings would cost \$2.00 per person as compared to \$0.20 with the present system.

Warren Seider reported that Fred Stults submitted his letter of resignation as Programming Board Chairman on August 8. Fred has also retired from DuPont. Fred was commended for the work he has done on the programming board. The committee moved to appoint Dick Mah as chairman

effective immediately.

Programming Area 15a (Systems and Process Design) reported that their program is set through 1981. Area 15c (Computers in Management and Information Processing) is planning sessions in Chicago and New Orleans.

PROGRAMMING

Fred Stults has submitted his resignation as chairman of the programming board effective August 8, 1979. Fred has done an excellent job as chairman and his services are deeply appreciated. Duties as programming board chairman are being assumed by Dick Mah. Dick is very experienced in the programming area and is an excellent choice as programming board chairman.

AREA 15a SYSTEMS AND PROCESS DESIGN

Dick Mah is retiring as chairman of Area 15a after having done a superb job. Jim Douglas (Chemical Engineering Department, University of Massachusetts, Amherst, MA 01003, 413-545-0705) is Dick's successor as chairman of Area 15a. The proposed programs for Area 15a through 1981 are given below.

Philadelphia - May 1980

Environmental Modeling
R. Stanfield (Exxon Research & Engineering Company)
H. Cole

Population Balances in Chemical Eng.
D. Ramkrishna (Purdue University)
H.K. Hulburt (Northwestern University)

Portland - August 1980

Special Purpose Computing Systems in Chemical Engineering
E.M. Rosen (Monsanto)
T.F. Edgar (University of Texas)

Use of Small Programmable Calculators in ChE Education
D.M. Himmelblau (University of Texas)
P.B. Kreiger (University of Washington)

Distributed Data Processing and Communications

T.I. Peterson (IBM)
T.M. Tayyabkhan (Mobil)

Chicago - November 1980

Computers in Process Design & Analysis
A.W. Westerberg (Carnegie-Mellon University)

Micro Computer Systems for ChE Education
J.D. Wright (Xerox Corporation)
P.A. Taylor (McMaster University)
(Coordinated with the session in Area 15b on Micro Computer Process Control Applications)

Improvements in Finite-Difference Methods

S. Churchill (University of Pennsylvania)
J.O. Wilbes (University of Michigan)

Houston - March 1981

Interface Between Design & Control
G. Stephanopoulos (University of Minnesota)

Optimization Theory & Applications
R.W. Pike (Louisiana State University)

Detroit - August 1981

ChE in the Manufacture of Computer Components
M. Tayyabkhan (Mobil Research & Development)

Modeling of Coal Conversion Processes

New Orleans - 1981

CAD Systems in ChE - Where are We?
E.M. Rosen (Monsanto)

Computers in Process Design & Analysis

AREA 15c
SYSTEMS AND PROCESS CONTROL

Area 15c is planning one session in Philadelphia and three in Chicago.

Philadelphia - May 1980

Applications in Process Control
M. Beaverstock (The Foxboro Co.)

Chicago - November 1980

Micro Processor Application in Process Control
J.D. Wright (Xerox of Canada)
P.A. Taylor (McMaster University)

Recent Development in Control System Design & Estimation (2 Sessions)
G. Stephanopoulos (University of Minnesota)
E. Bristol (The Foxboro Co.)

1980 JOINT AUTOMATIC CONTROL CONFERENCE

AIChE is one of the societies sponsoring the 1980 JACC which is to be held in San Francisco on August 13-15, 1980. A call for papers has been issued. Interested parties should contact the AIChE conference representative Dr. George Stephanopoulos, Department of Chemical Engineering, University of Minnesota, Minneapolis, MN 55455.

FOUNDATIONS OF COMPUTER-AIDED CHEMICAL PROCESS DESIGN

July 6-11, 1980

The CAST Division and the Engineering Foundation will sponsor a conference entitled "Foundations of Computer-Aided Chemical Process Design", to be held at New England College, Henniker, New Hampshire, July 6-11, 1980. Serving as co-chairmen of the conference are Richard S. H. Mah, Northwestern University, and Warren D. Seider, University of Pennsylvania.

In recent years advances in this important field have been greatly stimulated by process energy conservation and efficiency enhancement, new coal gasification and liquefaction processes, and the changing raw material situation. These advances are reflected in the estimation of thermophysical and transport properties, equipment design, unit modeling, flowsheet analysis, etc. Even experts have found it difficult to keep abreast of the rapid pace

of development in all subfields.

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.

The preliminary program outline is as follows:

Sunday, July 6, 1980

3:00 p.m. - 9:00 p.m. REGISTRATION AND CHECK-IN

Monday, July 7, 1980

Morning Session NON-LINEAR ALGEBRAIC EQUATIONS
2:00 p.m. - 5:00 p.m. AD HOC SESSIONS
Evening Session THERMOPHYSICAL AND TRANSPORT PROPERTIES

Tuesday, July 8, 1980

Morning Session NON-LINEAR PROGRAMMING
2:00 p.m. - 5:00 p.m. AD HOC SESSIONS
Evening Session PROCESS MODELING & ANALYSIS I - MULTITAGED TOWERS

Wednesday, July 9, 1980

Morning Session ORDINARY & PARTIAL DIFFERENTIAL EQUATIONS
2:00 p.m. - 5:00 p.m. AD HOC SESSIONS
Evening Session PROCESS MODELING & ANALYSIS II - Reactors

Thursday, July 10, 1980

Morning Session RECENT ADVANCES IN FLOWSHEETING PROGRAMS
2:00 p.m. - 5:00 p.m. AD HOC SESSIONS
Evening Sessions PROCESS SYNTHESIS

Friday, July 11, 1980

Morning Session SUMMARY & OVERVIEW

Engineering Foundation Conferences were established in 1962 to provide an opportunity for the 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 later.

To obtain an application, or more information, contact the Engineering Foundation, 345 East 47th Street, New York, NY 10017. Telephone: (212) 644-7835
Cable: ENGFOUND NEW YORK, Telex: 236411 IEEE UR.

CONTINUING EDUCATION

Engineers who are active in the area of computing and systems technology face a formidable continuing education challenge. Acquiring a current understanding of hardware and software developments in the face of such a rapidly developing technology is a problem that CAST is trying to address. One very effective way of meeting this challenge is through the AIChE Continuing Education Program. CAST is soliciting input on continuing education from its membership. If you are

willing to present a continuing education course or have some constructive comment to offer, please contact:

Richard Hughes
Engineering Expt. Station
University of Wisconsin
1500 Johnson Drive
Madison, WIL 53706
608-263-1602

COMPUTERS & CHEMICAL ENGINEERING
AN INTERNATIONAL JOURNAL

Since early 1977, a new journal has been receiving favorable attention from chemical engineers interested in computing and applied mathematics. With the appearance of Volume 2, Number 4 in June, the published material will amount to 40 papers, 5 short notes, and 2 reviews. Contributions have appeared in each of the major areas identified in the journal announcements:

- Process synthesis, analysis, and design
- Dynamic analysis and control of chemical processes
- Design methods for chemical engineering equipment, including chemical reactors, distillation columns, extractors, etc.
- Applications of computing and numerical analysis in chemical engineering science

The subjects covered and the authors involved are further exemplified by the following Table of Contents for Volume 2.

Plans for the journal include a regular feature on "Algorithms and Programs". This is intended to carry descriptions and listings of algorithms and programs for general use in chemical engineering calculations, which have received prior testing by members of CAST. Arrangements have been made to store the tested source programs at AIChE headquarters, for reproduction at nominal cost. As yet, none of these algorithms or programs have been published, but the Feature Editor, Charles Ware, has examined several candidates, and expects eventual success.

Volume 3 will include a special, combined issue containing papers of permanent significance from C.A.C.E. '79, the 12th

Symposium on Computer Applications in Chemical Engineering of the European Federation of Chemical Engineers, held at Montreux, Switzerland in April. The Co-chairman of the Symposium, Professor D. W. T. Rippin, is acting as Guest Editor for this issue. It is hoped that 40 to 50 papers can be published, including:

M DENTE, E RANZI, A G GOOSSENS, Rigorous Prediction of Olefin Yields from Hydrocarbon Pyrolysis through Fundamental Simulation Model (SPYRO)

H EGLY, V RUBY, B SEID, Optimierung Diskontinuierlicher Rektifikationen mit überlagerten Reaktionen

A MAUDERLI, D W T RIPPIN, Production Planning and Scheduling for Multi-Purpose Batch Chemical Plants

F BERGER, F A PERRIS, FLOWPACK II - A New Generation of System for Steady-State Process Flowsheeting

L B EVANS, J F BOSTON, H I BRITT et al, ASPEN: An Advanced System for Process Engineering

M TSUBAKI, R L MOTARD, Data Based Process Simulation

G STEPHANOPOULOS, Y ARKUN, M MORARI, A Unified Approach to the Synthesis of Control Structures for Complex Chemical Plants

W R JOHNS, T A VARDAS, Optimal Process Design and Selection

R K MALIK, R R HUGHES, Optimal Design of Flexible Chemical Processes

The special issue will also contain a summary by Prof. Rippin and the comments of the rapporteurs:

R W H SARGENT, Flowsheeting

O A ASBJORNSEN, Project Evaluation Safety and Reliability

R MOTARD, Process Synthesis

M RENARD, The Design and Operation of Batch Processes

In spite of the size of this special issue, there will be at least one regular issue in Volume 3. Manuscripts should follow the requirements given inside the back cover of each issue of the journal, and may be sent to the Editor:

Richard R. Hughes
University of Wisconsin
1500 Johnson Drive
Madison, WI 53706

Descriptions of algorithms and programs may be sent directly to the Feature Editor:

Charles H. Ware, Jr.
Commercialization Insights
33 Sandi Drive
Poughkeepsie, NY 12603

(Do not send program card decks or tapes until requested.)

A special subscription price of \$30.00 is available for individuals connected with an institution whose library has already subscribed. All AIChE members may obtain subscriptions for their personal use at a cost of \$20.00 per year. All subscription inquiries should go to:

The Subscriptions Fulfilment Manager
Pergamon Press Ltd.
Headington Hill Hall
Oxford OX3 0BW
ENGLAND

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OFF-LINE REVIEWS BY JOE ZEMAITIS

Having missed the last issue of the CAST newsletter because of a long illness and the resulting work backlog, there are several books which I would like to mention in this issue. But before discussing some of the basic texts, I want to call your attention to what is becoming a word-of-mouth best seller. That is an outstanding book by Professor Douglas R.

Hofstadter entitled "Gödel, Escher, Bach: an Eternal Golden Braid", Basic Books, Inc., New York (1979), 777 pages, \$18.50.

This book by a young computer scientist adapts the musical style of Bach in creating dialogues based on the structure of Bach's fugues, preludes, canons, and inventions to explore in a manner reminiscent of Lewis Carroll the basic nature of our thought process. Drawing heavily on recent work in artificial intelligence and Gödel's Theorem:

"All consistent axiomatic formulations of number theory include undecidable propositions."

Hofstadter explores all forms of symbol manipulating systems from mathematical logic and computer science to the thought process of the human mind.

Some idea of the contents of this magnificent book may be gained by sampling some of the chapter headings:

"Chapter V: Recursive Structures and Processes

Chapter VI: The Location of Meaning

Chapter VII: The Propositional Calculus

Chapter VIII: Typographical Number Theory

Chapter IX: Mumon and Gödel"

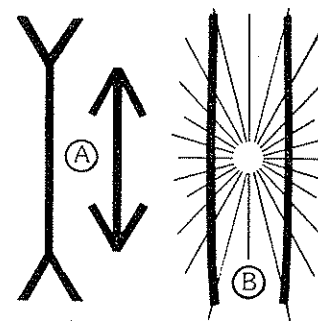
In this chapter, Hofstadter attempts to talk about the ideas of Zen Buddhism drawing on the commentaries of Mumon, a Zen monk. He shows that in a way, Zen ideas bear a metaphorical resemblance to some contemporary ideas on the philosophy of mathematics.

Like well known paradoxical drawings of Escher and the music of Bach, Hofstadter's book develops into a strange loop and turns back on itself, ending by beginning. This book is an excellent work of both art and science and well worth digging into time and again. If your bookstore doesn't have it, order a copy now.

Along more conventional lines I wish to

briefly mention a few other books, in particular a new edition of "A First Course in Numerical Analysis" by Anthony Ralston and Phillip Rabinowitz, McGraw-Hill, New York (1978), 566 pages. This book is both a basic introduction and an advanced text filled with excellent discussions on various numerical techniques covering linear algebraic equations, nonlinear algebraic equations, ordinary differential equations, functional approximations, etc. Being an introduction at times there is insufficient detail, as for example in the section on the numerical solution of stiff ordinary differential equations; however, an excellent annotated bibliography at the end of each chapter discusses the recent works of a more advanced nature and indicates which the authors feel should be explored. This bibliography alone, makes this book extremely useful and makes me wish that they had covered partial differential equations.

Finally, some brief comments on a book due to be out in December or January, that is entitled "Computer Applications to Chemical Engineering Process Design and Simulation" R. G. Squires, ed. ACS Symposium Series, Washington, (1979). This book will consist of the complete set of papers delivered at an excellent symposium in Washington in September, 1979. Beginning with several state of the art reviews of the primary areas of computer applications, the papers present a wide selection of new approaches to computation techniques, optimization, and control of processes and ends with several selected papers discussing the modeling and simulation of industrial processes. It is of some note that many if not most of the authors are members of CAST. It also leads to the question of why isn't CAST working with the AIChE to develop AIChE Symposium Series based on sessions presented at national meetings? During the past few years, there have been several symposia that would have benefited from collective publication in one source rather than the current dispersive practices observed.



You may figure you beat us to the punch on this one. You may be thinking, "Can't fool me with that old one. Those lines (A) are equal in length, and the other ones (B) are straight, not curved like they look. It's just an optical illusion that makes them look different."

Well, surprise! The arrow shaft on the left really is longer than the other one. And those lines really are curved!

Mistress Mary was the possessor of a diminutive and immature specimen of the genus (*OVIS aries*), a wool-bearing, ruminant quadruped.

The shaggy and agglomerated filaments, constituting in their collective capacity, its natural outer covering, presented to the vision a surface that rivals the immaculate areas of crystallized vapor which characterize a winter's landscape.

To whatsoever locality, contiguous or remote, whither Mary's vagrant fancy, or parental mandate, impelled her, this immature specimen of the genius *OVIS* could be counted upon, with absolute and complete certainty, to accompany her.

- Author Unknown