
NEWSLETTER

COMPUTING AND SYSTEMS
TECHNOLOGY DIVISION



SEVENTY-FIVE YEARS OF PROGRESS

AMERICAN INSTITUTE
OF CHEMICAL ENGINEERS

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PUBLICATION BOARD'S MESSAGES

by Dr. Edward Gordon
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One disadvantage of the increased size of the CAST Newsletter is the additional effort it takes to prepare the material for publication. Since the effort is performed almost entirely by volunteers, there is a greater opportunity for unplanned delays when crises arise in the jobs we are being paid for. As a consequence, the Spring 1984 issue was mailed just before the Anaheim National Meeting in May. This Fall issue has not done as well and it is being sent out after the San Francisco Meeting. One small benefit is that the list of Microfiche for that meeting is included.

Starting January 1, 1985, Professor Peter Rony will take over responsibility for the Newsletter and the CAST Publications Board. Peter has been the editor for the IEEE Computer Society publication called Micro for the past two years. The next item in this Newsletter is a message for the CAST membership from your new editor.

In this issue, there is a History of computers from a Chemical Engineering point of view. This summary is intended as background for our younger members to help them understand the enormous changes which have occurred in the past forty years as Computer-Aided Chemical Engineering has become a reality. In the previous issue, Ted Leininger covered the history of the Machine Computation Committee which spawned CAST.

Your new editor has provided some reflections on a recent visit to Japan. Irv Rinard, the Area 10b Chairman, covers what probably is the largest effort to date in applying the ASPEN program.

by Prof. Peter Rony, Virginia
Polytechnic Institute

The CAST Executive Committee elected me as Chairman of the Publications Board for the two year period, January 1985 -- December 1986. I am honored by this appointment, and will try to do my best to sustain the hard work, momentum, and imagination provided by Ed Gordon during his term in office.

To those of you who do not know me, my qualifications include: (a) I have been Editor-in-Chief of IEEE MICRO, a publication (24,000 subscribers) of the IEEE Computer Society, during the period January 1983 -- December 1985; (b) I have benefited from my association with competent IEEE Computer Society personnel in the publications area, among whom include True Seaborn, IEEE MICRO; (c) I believe that the editorial process is fundamental for a professional organization; and (d) I had the foolishness to be vocal about my concerns for the AIChE flagship magazine, CEP, which I felt has neither presented the totality of our profession effectively nor been competitive with other flagship magazines such as, for example, IEEE Spectrum and IEEE CS Computer. It is of interest to note that Computer magazine started as a newsletter, much like the CAST Newsletter, about fifteen years ago.

Ed has been publishing and mailing the Newsletter from his office in Irvine, California. With the change of the AIChE staff in New York, the CAST Executive Committee desires to have the AIChE headquarters participate more strongly in the publication of the magazine. CEP has a new publisher, Diane Foster, and a new editor, Agnes K. Dubberly, who have exciting plans for the magazine. I look forward to the collaboration of the CAST Division with them.

(CONTINUED ON PAGE 24).

1984 CAST AWARDS

The Computing in Chemical Engineering Award is given in recognition of outstanding contributions in the application of computing and system technology to chemical engineering. G.V. (Rex) Reklaitis received his B.S. degree from the Illinois Institute of Technology and his Ph.D. degree from Stanford University. Rex has spent a year in Switzerland as a NSF post-doctoral fellow and a semester in Lithuania SSR as Senior Fulbright lecturer. He has taught at Purdue University for 12 years. He is the author/co-author of 2 books, co-editor of an ACS Symposium Series Volume, and of an AIChE Symposium Series Volume, all in the areas of computer-aided design, optimization, and flowsheeting. He is the author of a number of research papers in these fields, focusing most recently on computer aids for batch/semi-continuous process design and analysis as well as on applications of computer graphics. He is currently Vice-President of CACHE Corporation and has been a Director of the CAST Division.

The Ted Peterson Award is given for a paper co-authored by a student. Chau-Chyun Chen is Principal Engineer at Aspen Technology. His areas of specialty are applied thermodynamics and computer-aided process simulation. He has published and presented many technical papers in the fields of enzyme technology, electrolyte thermodynamics, and process simulation. He holds a B.S. degree in chemistry from National Taiwan University and M.S. and Sc.D. degrees in Chemical Engineering from the Massachusetts Institute of Technology. He is a member of AIChE, ACS and Chinese Institute of Engineers, U.S.A.

Both awards were presented at the CAST Awards banquet at the AIChE meeting in San Francisco. Professor Reklaitis gave a talk entitled, "Prospects for Computer-Aided Batch Process Engineering".

CAST AWARDS SOLICITATION OF NOMINATION

Please use the form on the next two pages to submit your nomination to Jeff Sirola by March 31, 1985. Use a separate copy of the form for each nomination.

Computing in Chemical Engineering Award

This award is given to recognize outstanding contributions in the application of computing and systems technology to Chemical Engineering. It is normally awarded annually and consists of a plaque and a check for \$1500. Funding for the three years (1982-84) has been provided by Simulation Sciences of Fullerton, California, and Intergraph Corporation, Huntsville, Alabama. The 1983 Awardee was Arthur W. Westerberg of Carnegie-Mellon. The 1982 Awardee was Lawrence B. Evans of ASPEN Tech. formerly Professor of Chemical Engineering at MIT and leader of the ASPEN Project at MIT. The 1981 Awardee was Richard S.H. Mah, Professor of Chemical Engineering at Northwestern University. The 1980 Awardee was Brice Carnahan, at the University of Michigan. The 1979 Awardee, Richard R. Hughes at the University of Wisconsin, was the first recipient of the award.

TED PETERSON STUDENT PAPER AWARD

This award is given to an individual for published work in the application of computing and systems technology to Chemical Engineering. The work must have been done by the individual while pursuing graduate or undergraduate studies in Chemical Engineering. The award consists of \$500 and a plaque and is normally awarded annually. This is a new award and the first award was made in 1983 at the Diamond Jubilee Meeting in Washington, D.C. It is currently being supported by IBM and ChemShare, Inc. The 1983 winner was Carlos E. Garcia of Shell Development in Houston. He was a student at University of Wisconsin - Madison.

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

1985 AWARD NOMINATION FORM*

A. BACKGROUND DATA

1. Name of the Award _____ Today's Date _____

2. Name of Nominee _____ Date of Birth _____

3. Present Position (exact title) _____

Address _____
Institution or Company City and State Zip

4. Education:

<u>Institution</u>	<u>Degree Received</u>	<u>Year Received</u>	<u>Field</u>
_____	_____	_____	_____
_____	_____	_____	_____
_____	_____	_____	_____
_____	_____	_____	_____

5. Positions Held:

<u>Company or Institution</u>	<u>Position or Title</u>	<u>Dates</u>
_____	_____	_____
_____	_____	_____
_____	_____	_____
_____	_____	_____

6. Academic and Professional Honors (include awards, memberships in honorary societies and fraternities, prizes) and date the honor was received.

7. Technical and Professional Society Memberships and Offices

8. Sponsor's Name and Address _____

Sponsor's Signature _____

* A person may be nominated for only one award in a given year.

B. CITATION

1. A brief statement, not to exceed 250 words, of why the candidate should receive this award. (Use separate sheet of paper.)
2. Proposed citation (not more than 25 carefully edited words that reflect specific accomplishments).

C. QUALIFICATIONS

Each award has a different set of qualifications. These are described in the awards brochure. After reading them, please fill in the following information on the nominee where appropriate. Use a separate sheet for each item if necessary.

1. Selected bibliography (include books, patents, and major papers published.)
2. Specific identification and evaluation of the accomplishments on which the nomination is based.
3. If the nominee has previously received any award from AIChE or one of its Divisions, an explicit statement of *new* accomplishments or work over and above those cited for the earlier award(s) must be included.
4. Other pertinent information.

D. SUPPORTING LETTERS AND DOCUMENTS

List of no more than five individuals whose letters are attached.

Name	Affiliation
1.	
2.	
3.	
4.	
5.	

Please send the completed form and supplemental sheets by March 15, 1985 to the CAST Division Awards Chairman, Dr. Jeff Sirola, Tennessee Eastman Company, Kingsport, TN 37664

range of technological areas. A reading of Reischauer's "Japan The Story of a Nation" indicated that such a feeling has not been typical in post-war Japan. But it exists today, and it means that we should be aware of and sobered by, the competitive pressure that Japan will exert in many "high tech" areas ranging from megabit semiconductor memories to nuclear reactors. As a consequence of my visit, I developed a greater appreciation of and respect for what they have accomplished during the last twenty years, and what they plan to accomplish in the next twenty. The United States has every reason to be worried about the Japanese industrial challenge to its leadership.

At NEC, through the kindness of Mr. Kiyoshi Emi, I was able to tour their model office building (in Abiko) that exhibits state-of-the-art electronic office automation technology. Thin conductors under rugs. High-speed fiber optic information buses in the walls. Mechanical conveyors for documents throughout the building. A teleconferencing room that permits exchange of visual images (from electronic cameras, electronic tablets, and electronic blackboards) from Abiko to New York via satellite. Most impressive.

At Mitsubishi, I had the opportunity to observe development work on low-cost robots. One of the engineers was out of school only a year, and the other, at a different site, had about ten or more years of experience. What impressed me was that such engineers were responsible for the entire design of their respective robots: mechanical, microcomputer, interface electronics, and robot operating system software. The Japanese had a word for such an endeavor: mechatronics. There was strong product orientation, and a single individual was identified with a single product. I am not an industrial or manufacturing engineer, but my sense of American education is that we do not instill product orientation in our students as do

the Japanese. Also, the mechanical skills of undergraduate engineers are weaker than they were 30 years ago; many, if not most, U.S. engineering students no longer have experience in machine shop. The Japanese whom I met were very product oriented: define it, develop it, and market it. For a new engineer fresh from a university, a successful product would have annual sales of, for example, \$1,000,000 to \$2,000,000 and would have a lifetime of at least several years.

A final topic is the matter of sales of Japanese personal computers in the United States. I frequently asked representatives of the companies I visited, How are your personal computer sales doing in the U.S.? The answer: To date, such sales have not met expectations for reasons which they did not completely understand. The weak American reaction to their computers, which they considered to be competitive with the IBM PC and its clones, has come as a surprise--an exception, perhaps temporary, to the Japanese success stories in cameras, video tape recorders, watches, automobiles, and portable radios. When the questioning was reversed and I was asked if I would purchase a Japanese computer, my answer was no unless the PC was very inexpensive or novel. When asked to elaborate, I explained that I had no confidence that standard third party hardware and software would be available for a Japanese PC. I did not want to become stuck with a machine that was poorly supported by the U.S. computer industry.

I would like to thank my many Japanese hosts, who, in addition to the individuals mentioned above, included Mr. Osamu Takahashi, Mr. Tadashi Kurachi, Mr. Shoji Hiroe, Mr. Tohru Haegawa, Mr. Teiichi Tanaka, Mr. Fumihiro Nakamura, Mr. Akira Naito, Mr. Toyooki Taniguchi, and others. Our conversations enriched my appreciation of your country.

HISTORY OF COMPUTERS

from a Chemical Engineering Point of View

by Dr. Edward Gordon Fluor Engineers Inc.

In the previous issue of the CAST Newsletter, Ted Leininger presented an excellent history of the A.I.Ch.E Machine Computation Committee (MCC) which was the predecessor to CAST (1). That paper presents a review of the dramatic changes in the role of computers in Chemical Engineering over the past forty years. That review provides some background which explains the timing of many of the MCC events.

WHERE WERE WE FORTY YEARS AGO?

Forty years ago, there were very few digital computers in the world. The slide rule was the most commonly used aid to Chemical Engineering calculations. There were a few calculations like tray-to-tray distillation calculations which required more precision than a slide rule could provide (2). For those calculations, a mechanical desk calculator which typically could handle 8 or 10 digit numbers was used in 1944. Those calculators were limited to the same four functions (addition, subtraction, multiplication, and division) (3) that an inexpensive pocket calculator performs today with much less noise and effort.

There were a number of mechanical analog computers available. They had been used for solving simultaneous equations back in the twenties. Network flow was simulated electrically as far back as 1925. Their usefulness in solving differential equations was known in 1931. Bell Labs started work on electronic analog computers in the mid-thirties (4).

The Sorter for punched cards was invented by Hollerith for processing of the data from the 1890 U.S. Census. It provided some very effective tabulating capabilities which made it possible to complete processing of the data before the next census (5). Various printing and logical capabilities were added as those devices evolved into Accounting Machines. In the late thirties, IBM introduced their Model 601 Calculator which did multiplications much like a desk calculator.

Before that, multiplications were performed by repeated additions without a convenient mechanism for shifting to the next decimal digit. The IBM Model 602 which came along a few years later was also capable of performing divisions.

Accounting Machines were computational devices which performed relatively simple manipulations of the numbers or characters they read from punched cards. The results could be punched into the same card, into another card, or printed (6). Those manipulations were much like today's subroutines and in many ways Accounting Machines behaved like computers. The usual Accounting Machine had very limited data storage within the machine, typically much less than 100 digits. A few unusual installations had rather substantial capabilities for their time.

The best known of the sophisticated relay based machines is the monster (Automatic Sequence Controlled Calculator) which IBM built for use at Harvard University starting in 1938 (7). Zuse built relay based computers for the Germans which received much less attention (8). Perhaps the most important military application was the British work on Cryptography (9).

The first electronic digital computing device was initiated in 1938 by Atanasoff and Berry for the solution of up to 30 simultaneous linear equations (10). For all of these machines, programming was done by plugging wires into a Control Panel (11). Thus, it was far more difficult to program than with any computer in use today. I don't know of any published accounts of applications of computers in Chemical Engineering before 1944. However, the situation changed drastically very soon thereafter.

ACCOUNTING MACHINES 1944 - 1954

Although major advancements were made in computer development (12), they had very little impact on Chemical Engineering in that decade. The major advances in Chemical Engineering computations came from applications of Accounting Machines. Those machines were relatively common particularly in the larger companies. Since most accounting operations are cyclical, there were times in the various accounting cycles when the machines were idle.

A number of Chemical Engineers became aware of the availability of those machines on a non-interference basis and managed to penetrate the language barrier. In addition, the capabilities of the IBM Calculators were substantially improved. The Model 602 was replaced by an advanced version, the Model 602A and before long the arithmetic was done using vacuum tubes, by the IBM 603 and 604. Furthermore, these applications started to attract attention and IBM sponsored a number of symposia (13).

A 1950 article by Rose and Williams at Penn State describes how they did distillation calculation using an IBM 604 (14). A year later Opler and Heitz described their doing a six component system distillation on an IBM 602A (15). However, distillation calculations were not the only ones requiring more precision than a slide rule could provide. Data analysis via regression also required greater precision.

In 1949, I became aware that the facility I was working in had an IBM 601 and I was spending most of my time doing data analysis. After much difficulty, I was finally able to get our Accounting Machine expert to wire a Control Panel which I could use to generate the crossproducts needed for regression. The 601 took two three digit numbers which it read from the punched card and punched their product in to the same card. These products were then summed by a 402 Tabulator to generate the matrix of coefficients representing the normal equations. I was fortunate that we had a Mass Spectrometry group who spent most of their time solving sets of simultaneous equations to generate useful analyses from the measurements. They could solve my set of equations in about 20 minutes. Since neither the 601 nor the 402 could divide, it was impractical to try to get either one to solve the equations. The key point is that in spite of the many frustrations involved and the many steps it took to generate the desired results, in six months I was able to come up with more and better correlations than I had in the previous four years using graphical data analysis methods.

As scientific applications of Accounting Machines became more common, IBM then decided that they should get into computers. They also made available a data storage box for use with the IBM 604 Calculator and a 402 Tabulator. They called that configuration a Card Programmed Calculator (CPC) and it was very popular in the early fifties (16). Those boxes had a storage capacity of fifty 20 digit numbers for a total of one thousand digits, a major step forward.

There was relatively free exchange of ideas and techniques and Prof. Rose and associates started a series of review articles on Computers, Statistics, and Mathematics (17).

MOVING UP TO COMPUTERS 1954 - 1964

Although the first Univac Computer was delivered to the Census Bureau in 1951 (18), digital computers not based on accounting machines did not have much impact on Chemical Engineering until they were more common. Relatively few were sold and they were used primarily for business type applications. The more important early computers in Chemical Engineering, were the ElectroData (Burroughs) 205, IBM 704 and IBM 650 which were first delivered in 1954, 1955, and 1956 respectively.

Early computers were classified as large, medium and small based on price. One hundred thousand dollars was the lower limit on medium and 750 thousand the upper limit (19). The IBM 704 was in the large class so its Chemical Engineering application came largely from the Oil and Chemical Companies. The Engineering Companies favored the 205 over the 650 even though both were in the medium price range. The 205 had 4080 ten digit words of data and program storage on its drum. That corresponds to 20.4K bytes which is small by today's standards even for a personal computer. The 650 was even smaller when it was introduced though later models did have 4000 words of storage.

When these computers were first delivered, they did not have any assemblers or compilers. Effectively, programming was done in absolute machine language. That was not too difficult for the 205 because it was a decimal machine and it used a single address per command structure. In due time, programming aids were developed (20).

When Fortran was first described at a computing conference, it was described as a language developed for those mathematicians who were unwilling to learn machine language so they could write their own one-shot programs for the IBM 704 without bothering the programmers (21).

Fortran had very limited usage on the first generation medium priced computers, although it made quick inroads on the larger IBM machines. Univac had their own compiler. Ultimately, versions of Fortran were developed which could be used efficiently on medium priced machines (22). However, by then the first generation machines were largely obsolete. Tube machines required much more maintenance than the transistor machines of the second generation.

Computer Graphics were largely limited to CalComp plots of graphic output or Tektronix CRT displays. A few were using light pens for graphic input. The technology goes back to the Whirlwind Project at MIT which was started in 1947 (23). One area which received much attention was Air Traffic Control and the development activity was applied in the SAGE system. The latter used a monstrous array of first generation computer hardware in a project which required reasonably good reliability (24). The modern approach to interactive graphics was under development with the SKETCHPAD project at MIT being the best known effort (25).

The most spectacular computer development effort in this time interval was the Stretch Computer Project. Its goal when it started in 1956 was one hundred times the performance of an IBM 704. It was soon found that a ten fold improvement in basic circuit speed was the best they could achieve with the technology of that time and a six-fold improvement in memory performance. Thus, they didn't quite make their goal except for double precision floating point operations and mesh type calculations where their look ahead features were quite effective (26).

Although it was started in the first computer generation, it was completed after the second generation was on the scene and it carried a second generation model number, 7030. Because it didn't quite make its performance goal, its selling price was well below IBM's cost. That led to a statement attributed to Tom Watson that if they sold enough of that computer, the losses could be sufficient to drive IBM out of business. The design advances were adapted to raise the performance of the 7094 model over its predecessor, the 7090, enough to offer a more favorable cost-performance ratio (27) and many customers switched to the less expensive 7094.

A more practical supercomputer was the CDC 6600 which was started in 1960. Their first machine was delivered in 1964 (28). With faster circuitry than Stretch used and greater emphasis on number crunching, it was a commercial success. CDC and their Chief Systems Designer, Seymour Cray quickly gained undisputed leadership in supercomputers (29).

DEVELOPING MAJOR SYSTEMS 1964 - 1974

Certainly the most popular computer in the third generation is the IBM 360 series, although for a short while there were doubts. The 360 series was a complete break from all members of the IBM 7000 series second generation machines. The IBM 7000 scientific machines used a 36 bit word which was also interpreted at six 6-bit characters (30). That led to the IBM seven track tapes.

In contrast, the IBM 360 series was based on four 8-bit bytes each of which can represent a character (31). Thus, the 360 machines used nine track tapes. This essentially complete incompatibility was a traumatic experience for IBM customers. However, as usual, IBM provided ample program conversion support and successfully weathered the storm.

Many companies which placed heavy emphasis on their engineering calculations ended up with either a 6000 series CDC computer or a UNIVAC 1108 type machine for those calculations. There were significant differences between the CDC and UNIVAC versions of Fortran but even larger differences between those versions and the IBM Version (32). However, for documentation of algorithms in technical journals, ALGOL was the standard language (33). Since very few of the programmers knew ALGOL, this made the algorithm literature much less useful for engineering applications.

From a Chemical Engineering calculation point of view, the key point is that these larger and more powerful computers made the development of major Flow Sheet Simulation Programs practical. Computer Aided Chemical Engineering became a reality. Previously, ability to perform such calculations was much more limited both in terms of what could be done as well as how many people were able to do them. Ed Rosen presented an insider's view of the development of FLOWTRAN (34). Most major Oil and Chemical Companies as well as Engineering and Construction firms were developing their own major systems.

In the same time frame, independent software vendors were developing their own systems primarily used via Service Bureaus. However, the resources required normally exceeded those an independent vendor could put together and they had much difficulty competing with in-house systems unless very specialized technology was involved. Interactive computing was quietly growing also.

CONTINUED GROWTH 1974 - 1984

With continued growth in the usage and capabilities of the computers and the software packages, there was also continued growth in the cost of supporting and maintaining these systems. In addition, major cooperative efforts such as ASPEN and various Design Institutes made the computational technology more readily available (35,36). As a consequence, the major packages from independent software vendors started to become more competitive in capabilities with the large in-house systems.

With the continued shrinking of computer circuitry based on large scale integration, it became feasible to put an entire CPU on a chip (37) and Microcomputers became available. Minicomputers was the name given to what formerly were called Medium sized computers. With the progress in circuitry the Minicomputers were competitive in performance with the large main frames of just a few years earlier vintage. One of the more important applications of those Minicomputers is Computer-Aided Design (CAD) which has been defined as the use of interactive graphics programs to develop diagrams, parts lists and working drawings (38).

As CAD developed and proliferated, the capabilities were extended to the utilization of the CAD information in Numerically Controlled manufacturing devices to make Computer Aided Manufacturing (CAM) much more common. Tying the CAD system with Process Simulation and Data Base Managers is leading to Computer Aided Engineering (CAE). The progress has been especially spectacular in computer chip design (39). There are so many details to contend with and wiring lists have been in widespread use for many years.

However, Process Design differs in many fundamental ways from Chip design and progress in that kind of CAE has been much slower (40) even though we are getting close to practical Ch.E. work stations. Relational Data Bases do offer much promise (41) and Local Area Networks (LAN) are providing communication capabilities commensurate with work station needs (42).

One byproduct of the much greater use of large scale integration computer chips is the gain in reliability. The first computer I used required four hours per day of hardware maintenance in addition to about eight hours every weekend. When the cause of a program failure was not an obvious program or input error, there was a fifty percent chance that the fault was a hardware malfunction. Today, the amount of self testing which is automatically performed is sufficient to make undetected hardware malfunctions an extremely unlikely cause of software failures (43).

Consequently, Microcomputer reliability is now sufficient that they are being widely used in Process Control Systems. With the much greater computational capability now available to Control Systems, major changes in control philosophies are now practical and receiving serious attention (44).

WHERE TO FROM HERE

The strong trends now underway are in some ways incompatible so it is difficult to predict where the current trends will be taking us. There is much effort being devoted to CAE for Process Design with the traditional Ch.E. software vendors playing a minor role and the CAD software vendors being dominant. However, data base utilization is a critical part of the major gains anticipated and the current CAD systems have their own specialized and relatively inflexible data bases.

Microcomputers are rapidly becoming much more powerful and widely used. Yet the primary applications are Word Processing and Spread Sheet applications (45). Software development costs inhibit the development of more specialized programs with a relatively limited market. To me, the most logical direction is distributed systems where the Microcomputers do those tasks which they are most cost-effective for and large Mainframes continue to do what they do best. However, there are a number of major problems which need to be solved before distributed systems will be practical.

Widespread use of computers in Chemical Engineering education is anticipated because of the substantial benefits possible. The programming effort required may be less than the computational effort avoided (46).

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Great Plains ASPEN Model Project by by Dr. I.H. Renard Halcon SD Group, Inc.

In late 1983, the U.S. Department of Energy (DOE) contracted with the Halcon SD Group (HSD) of New York to develop a steady-state simulation model for the Great Plains Coal Gasification Plant. The model was to be developed using the ASPEN (Advanced System for Process Engineering) program developed for the DOE by the Massachusetts Institute of Technology. The plant, now in start up, is designed to produce 125 MM SCFD of substitute natural gas from the gasification of North Dakota Lignite. It was the DOE's intention to demonstrate that the ASPEN program could be used to provide useful simulation models of the plant.

The project involved five major activities. These were:

1. Physical properties evaluation and modeling,
2. Incorporation of a rigorous moving-bed gasifier model into ASPEN,
3. Cost estimation system evaluation and enhancement,
4. Development of flowsheet models for each of twelve plant sections from raw gas quenching through gas drying and compression, and
5. Case studies using the flowsheet models to determine sensitivity to key operating and design parameters.

PHYSICAL PROPERTIES

An evaluation of the pure component properties in the ASPEN data bank for the thirty five compounds required to simulate the Great Plains Gasification Plant (GPCP) was made. Both unary and temperature dependent properties were checked. The DIPPR (Design Institute for Physical Properties Data) data bank was used as the basis of comparison. It was found that the ASPEN data bank is for the most part reliable, its main problem being lack of documentation.

A second phase of the physical properties task was to establish parameters that could be used to predict the highly non-ideal vapor-liquid and liquid-liquid behavior in the process sections of the GPCP. The preferred approach would be to use a single equation of state to predict the phase equilibria for all sections of the plant. This was not possible. Some of the sections use activity coefficient models but the majority use the Peng Robinson equation of state modified for water.

GASIFIER MODEL

This task called for the incorporation into ASPEN of a rigorous model for a moving-bed gasifier. This was taken to mean a model that can predict results of changes in operating conditions on raw gas flow rate, composition, temperature; carbon conversion; and maximum solids temperature within the bed. An extensive survey of the literature yielded a number of gasifier models which appeared to be reasonable candidates for use in ASPEN. Of these, two models best satisfied the various evaluation criteria; one was developed at West Virginia University (WVU) by Wen and Desai and the other at the University of Delaware (UD) by Denn, Wei, and Yoon. Both have

been included in the gasifier unit operations block RGAS that has been incorporated into the DOE version of ASPEN. RGAS also includes a detailed devolatilization model. The UD model has been found to be easier to tune for a specific coal and somewhat more robust than the UWV model.

ASPEN COST MODELS

The ASPEN program contains within it a Cost Estimation System (CES) which estimates the purchase cost and utility consumption rates for major pieces of equipment in a process flowsheet. Each cost model contained in the CES was screened by making several stand-alone runs for equipment that had been purchased by HSD in the past. Where large discrepancies resulted between the price calculated by the CES and the actual purchase cost of the equipment, adjustments or changes to the CES models were made. These included either adjustment of the factors built into the models, incorporation of new cost correlations, or the development of new models altogether.

A new method for the estimation of commodity material and labor costs, which are associated with ME (Major Equipment) installation, has been developed and incorporated into the ASPEN CES. The original ASPEN method used cost-independent factors supplied by the user to determine these OE (Other Equipment) costs. The new method which has been implemented in ASPEN calculates OE factors from correlations based on purchased equipment cost.

PROCESS SIMULATION

Eleven ASPEN flowsheet models have been developed as part of this project. These include:

1. Oxygen Plant
2. Gasifier Quench, Shift Conversion, Gas Cooling, and Gas Liquor Separation
3. Rectisol (Acid gas removal)
4. Methanation
5. Gas Compression and Drying
6. Phenosolvan (Phenolics removal)
7. Phosam (Ammonia removal)
8. Cooling Tower
9. Methanol Plant (Rectisol solvent makeup)
10. Stretford (Sulfur recovery)
11. Steam Distribution

Almost all the technology in this list is proprietary. No detailed technical information such as heat and material balances or equipment design specifications were available from the licensors. All the flowsheet models are based entirely on publicly available information including that presented during the course of various public hearings as well as what is available in the literature.

The length of this article does not permit detailed descriptions of these models, their reliability, and the case study results obtained therefrom. Needless to say, the simpler the flowsheet, the more robust the model. For more details, refer to the more detailed summary paper given at the 1984 Pittsburgh Coal Conference ("A Steady-State Simulation Model for the Great Plains Coal Gasification Plant," by I.H. Rinard, S.S. Stern, M.C. Millman, B.W. Benjamin, K.J. Schwint, and D.R. Carnegie, all of HSD; L.E. Graham of DOE; and J.S. Dweck and M. Mendelson of JSD Consultants, Inc.). There are also a series of 20 topical reports for this project which should be available by the end of 1984.

ASPEN USER GROUP

The public ASPEN Users Group met on November 26, 1984 in conjunction with the National AIChE meeting in San Francisco, California. The next general meeting will be in Houston, Texas on March 24th.

Every November new officers are elected by the ASPEN Users Group. The new officers are:

Rita A. Bajura, Chairman
Department of Energy
Box 880
Morgantown, W. Virginia 26505
304-291-4714

Jim Henry, Vice Chairman
University of Tennessee at Chattanooga
Chattanooga, Tennessee 37402
615-755-4398

Trina J. Igelsrud, Secretary
Stearns Catalytic Corporation
Box 5888
Denver, Colorado 80217
303-692-4286

The other committee chairman appointed are:

Documentation and Training - Alfred Dyson
(205-729-3643)

Custody, Corrections and Enhancements -
Robert MacCallum, (918-660-3153)

Physical Properties - Martin Millman
(212-689-3000)

The tentative agenda for the March meeting is:

Monday, March 24 5:30 - 8:00 Business Meeting, Committee Reports, Technical talks.

The ASPEN Users Group has a 'bulletin board' supplied by Jim Henry from the University of Tennessee. The purpose of

this tool is to let every ASPEN Users Group member have access to information about the activities of the various Users Group Committees. Contact Jim Henry for instructions about how to implement the bulletin board.

DOE/METC has put the ASPEN documentation on the Wang system. The manuals need to be proofread for both spelling and conceptual errors. Anyone interested in helping out with this task please contact Rita Bajura or Alfred Dyson.

Stearns Catalytic Corporation has written a Condensed Users Manual for use in their company. It has been donated to the Users Group and for a reproduction/tabs/binder charge of \$52.00 they will deliver a manual to you. Contact either Alfred Dyson or Trina J. Igelsrud to place an order.

Due to the Great Plains Coal Gasification project, there has been a significant improvement in the Costing and Economics System. The changes have been incorporated into the public version and are available through NESC (National Energy Software Center).

The Physical Properties committee is comparing the unary parameters of the ASPEN data bank for the first 250 components with the values in DIPPR. This should be completed by the March meeting so the committee can recommend changes in the data bank to the Custody and Corrections committee. Anyone interested in helping with comparing DIPPR vs ASPEN PCD values should contact Martin Millman.

The ASPEN Users Group now has about 250 members. There is only one official member name and address list, the one maintained by the secretary. If anyone is interested in joining the group or wants information about any of the User Group's activities please contact any of the officers.

ORDERING MICROFICHE

Microfiche are available from AIChE Headquarters for at least one year after the meeting. Prices: \$2.50 per microfiche for AIChE Members, \$4.50 per microfiche for non-members. All sales are final - no returns are accepted. For additional information, call AIChE Technical Publications department (212) 705-7335

Washington, D.C., Oct. 30-Nov. 4, 1983

- Session 2 Chemical Engineering Education in the Next 25 Years: I-Undergraduate a,c: Fiche 51
- Session 9 Innovations In Applied Mathematics In Chemical Engineering b: Fiche 54
- Session 19 Chemical Engineering Education in the Next 25 Years: II-Graduate c: Fiche 30
- Session 21 History of Fractional Distillation b,f; Fiche 44; c: Fiche 45
- Session 26 Computer-Aided Process Analysis and Synthesis e,f: Fiche 5
- Session 33 Application of Computers in the Control and Management of Biological Processes-I a,b,c,f: Fiche 29
- Session 43 Computer Aided Engineering in the Chemical Process Industry-I Process/Project Evaluation b: Fiche 36; c,d: Fiche 35
- Session 44 Major New Directions in Process Control: I a,c: Fiche 43
- Session 50 Application of Computers in the Control and Management of Biological Processes-II a,c,f: Fiche 32; b: Fiche 33; d: Fiche 31

- Session 60 Computer Aided Engineering in the Chemical Process Industry II: Project Execution b,c: Fiche 51

Anaheim, CA May 20-23, 1984

- Session 5 Human Factors in Control System Design a,c,d: Fiche 17; b: Fiche 36
- Session 15 Microcomputers in the Laboratory a,f: Fiche 16; b: Fiche 36; h: Fiche 15
- Session 16 Process Modeling With Computers-I a: Fiche 1; c,d: Fiche 2
- Session 17 Microcomputers in Professional Practice: I b,d: Fiche 22
- Session 18 Software for Control System Design a: Fiche 3; b,d: Fiche 4
- Session 28 Microcomputers-Are They Useful in Project Management? d,e: Fiche 31
- Session 29 Process Modeling With Computers-II a,b: Fiche 7; c,d,e: Fiche 6
- Session 30 Microcomputers in Professional Practice: II b,c,d: Fiche 29
- Session 31 Software for Advanced Control a,b,d,e: Fiche 34; c,f: Fiche 22
- Session 41 Microcomputers in Education a: Fiche 12; b,c,d,f: Fiche 13
- Session 42 Computer-Aided Process Plant Design b,c,d,g: Fiche 12
- Session 43 Process Data Reconciliation and Rectification-I a,c,d: Fiche 19
- Session 44 Advanced Computer Control in Today's Refinery a: Fiche 37; b,c,d: Fiche 13
- Session 55 Process Data Reconciliation and Rectification-II a,c,d: Fiche 16

Session 56 Progress Toward Process Engineering Workstations a,d: Fiche 20; c: Fiche 31

Session 61 Pilot Plant Instrumentation and Control a,e: Fiche 9; b,c: Fiche 10

Philadelphia, Aug., 19-22, 1984

Session 43 Emulsion Polymers and Emulsion Polymerization - I Computer Modeling of Emulsion Polymerization a,b,d: Fiche 27

Session 53 Investment Decision Analysis Twenty-Five Years Later - Are the Numbers More or Less Helpful Now? - I a,b,c,d,e: Fiche 2

Session 54 Investment Decision Analysis Twenty-Five Years Later - Are the Numbers More or Less Helpful Now? - II a,b: Fiche 20

San Francisco, CA November 25-30, 1984

Session 8 Advances in Applied Mathematics b: Fiche 78; e,f: Fiche 108

Session 27 Advances in Numerical Analysis and Applications a,e,g: Fiche 47; c,d,f: Fiche 48

Session 42 Use of Computer Executive Programs in Plant Design b: Fiche 30

Session 45 Computer-Aided Design of Batch and Semicontinuous Processes a,d: Fiche 118; b,e: Fiche 72; c,f: Fiche 71; g: Fiche 119

Session 57 Pilot Plant Seminar I c,f: Fiche 54

Session 63 Computer-Aided Process Design and Analysis b,e: Fiche 41; c: Fiche 39; d: Fiche 29; f: Fiche 112

Session 76 Pilot Plant Seminar II a,c: Fiche 106

Session 82 Topics in Process Control I b,f: Fiche 68; d,e,g: Fiche 69

Session 88 Advances in Process Synthesis a: Fiche 54; b: Fiche 52; c: Fiche 107; d: Fiche 55; e: Fiche 53; f: Fiche 51

Session 91 Modeling, Simulation and Control in the Forest Products Industry-I a,b,c: Fiche 15; d,e,f: Fiche 113

Session 101 Topics in Process Control II a,c,f: Fiche 90; b: Fiche 10

Session 104 Combinatorial Optimization b:Fiche 110; c,d,f: Fiche 103; e: Fiche 109

Session 110 Modeling, Simulation and Control in the Forest Products Industry-II a,b: Fiche 73; c: Fiche 51; d,f,g: Fiche 34

Session 120 Modeling and Identification a: Fiche 45; c,d,e: Fiche 44; f: Fiche 43; g: Fiche 76

Session 123 Production Scheduling a,d,f: Fiche 94; c: Fiche 121

Session 131 Process Fault Detection and Diagnosis a,b,c,d: Fiche 26; e: Fiche 32

PROCESS SYSTEMS ENGINEERING 85, 31st MARCH -4th APRIL 1985, CAMBRIDGE, ENGLAND

PSE 85 will pick up the key themes of the first of the triennial series entitled PSE held in Kyoto in 1982, concentrating on OPERABILITY CONSIDERATIONS AT DESIGN STAGE: THE DESIGN OF FLOWSHEETS: AIDS FOR PLANT OPERATION and THE INFLUENCE OF NEW CAD TECHNOLOGY. While traditional subjects such as flowsheeting will be considered, the emphasis of this multi-national program will be very much on new topics and new directions.

PSE 85 is being organized by the Institution of Chemical Engineers on behalf of the European Federation of Chemical Engineering, in association with the Inter American Federation of Chemical Engineering, and the Asian Pacific Confederation of Chemical Engineering. As EFCE Event No. 313 this conference will continue a successful series of symposia held at the invitation of the EFCE Working Party on Computer Applications, taking place in Montreux in 1979, Heviz 1980, Vienna 1981, Antwerp 1982 and Paris 1983.

Registration will take place on the afternoon and evening of Sunday 31st March 1985. Technical sessions will be held from the morning of Monday 1st April to lunch time Thursday 4th April. The afternoon of the 4th will be devoted to technical visits and discussions.

MEETING SITE

Robinson College, Cambridge will be the venue for this multi-national event. An architecturally award winning complex Robinson College provides excellent conference facilities including accommodation of an exceptionally high standard. Particular attractive in the Spring, Cambridge offers a wealth of tourist interest to delegates and their partners.

TECHNICAL PROGRAM

The response to the Call for Papers has been excellent and many papers of a high caliber are still being considered by the Technical Papers Committee. A final program is not available at this stage, but an outline of the sessions and their technical content is given below. Complete details about papers and authors will be published in the Final Announcement which will appear during the early part of 1985. All papers selected for presentation will be published as No. 92 in the IChemE's Symposium Series.

OPERABILITY CONSIDERATIONS AT DESIGN STAGE

The primary theme of this session is the introduction of flexibility, dynamic resilience and controllability at the design stage and the influence of uncertainty upon them. New approaches are described which promise substantially improved plant operation resulting from the integration of these measures into the earliest stages of design, rather than trying to compensate for them if problems arise later.

THE DESIGN OF FLOWSHEETS

This session reports on the latest advances in the development of technology for flowsheet simulation and the optimum design of process networks. Various techniques are examined, including the potential application of Artificial Intelligence to such design. The handling of uncertainty in design information is also covered, as is the treatment of multi-phase systems.

AIDS FOR PLANT OPERATION

Papers under this heading cover training simulators, methods of detecting the primary causes of failure alarms and ways of monitoring plant performance, including the analysis of measured data. The session is particularly valuable in that it includes a number of contributions which report on industrial experience.

THE INFLUENCE OF NEW CAD TECHNOLOGY

The papers in this session describe the way in which new CAD technology is now becoming available for application. Ideas such as graphical input/output, data management and special methods for the use of Super-Computers are discussed here, as well as the possible exploitation of entirely new technology like Artificial Intelligence and Fuzzy Set Theory. The practical employment of this new technology is illustrated by descriptions of its introduction to and use in major industrial organizations.

POSTER SESSION

Papers best suited to a poster style presentation are included under this heading. Moreover, the session allows interesting and valuable papers, which cannot be accommodated within the confines of the above formal sessions, to be presented. The range of subjects is therefore diverse, from cost diagrams to program design methodologies.

EXHIBITION

The conference is expected to attract delegates throughout the field of PSE from all over the world. Floor space is available for approximately 12 companies to set up their own displays exhibiting products relating to process engineering CAD.

TECHNICAL PAPERS COMMITTEE

F.A. Perris (Chairman)
Air Products

P.S. Banks
BP

D. Depeyre
EFCE CAD Working Party Secretary

D.W. Gillings
Consultant

J.D. Perkins (Vice-Chairman)
Imperial College

J.W. Ponton
University of Edinburgh

M.L. Preston
ICI

G.V. Reklaitis
Purdue University, USA

L.M. Rose
ETH Zurich, Switzerland

R.W.H. Sargent
Imperial College

T. Takamatsu
Kyoto University, Japan

P. Winter
Prosyst Technology

FURTHER INFORMATION

Miss Julie Wearne, The Conference Section
The Institution of Chemical Engineers
165-171 Railway Terrace
Rugby, CV21 3HQ, UK

Tel: 0788 78214 - Telex 311780

"FOCAPD PROCEEDINGS"

Proceedings of the Second International Conference on Foundations of Computer-Aided Process Design held at Snowmass, Colorado in the Summer of 1983 are now available.

The week long meeting, sponsored jointly by the CAST Division of the AIChE and CACHE, with support from the National Science Foundation and Chiyoda Engineers and Construction Co., EXXON Research and Development Co., the Halcon SD Group, Monsanto Company, Olin Chemicals Corp., Process Simulation International, Shell Companies Foundation, Tennessee Eastman Co., and Weyerhouser Co.

Professor Arthur Westerberg (Carnegie Mellon University) and Dr. Henry H. Chien (Monsanto Co.) were the meeting co-chairman and served as editors of the Proceedings. The Proceedings (a hardbound book of more than 1000 pages) contain all 22 papers presented during the meeting, plus summaries of the discussions held during each session. The major sessions were:

1. Keynote (Expert Systems)
2. Overview and Outlook for Process Systems Engineering
3. Progress in Data Base Development
4. Computational Algorithms
5. Physical Properties for Design
6. Nonsequential Modular Flowsheeting
7. Design and Scheduling of Batch Chemical Plants
8. Complex Single Unit Design (columns, reactors)
9. Operability in Design
10. Contributed Papers (various topics),

The text is available at \$37.50 from:

Professor Brice Carnahan, Chemical Engineering Dept., The University of Michigan, Ann Arbor, MI 48109

MESSAGES' Continued from Page 1

Ten days spent in isolation in Blacksburg is insufficient time to develop a plan for the Newsletter during the 1985-86 period. A few thoughts have occurred that are worth sharing. First, I served a two-year apprentice period as Associate Editor-in-Chief of IEEE MICRO during 1980-1982. Such a period prepared me for my selection as Editor-in-Chief during the fall of 1982. Continuity in a publication is important, so I would recommend the appointment of several colleagues, one of whom would be the candidate for Chairman of the Publications Board in 1987-88.

Second, I invite all members of CAST to participate in providing contributions to our Newsletter. We shall continue what we already do well, shall offer our best material for publication directly in CEP, and shall experiment, with your assistance and guidance, with new ideas that have as their objective an expanded role for the CAST Publications Committee. We expect to "win a few, and lose a few" in our attempts to move the CAST publication activity forward, but hope to identify several innovations that will have lasting value.

Third, and finally, I will be on sabbatical leave at the University of Delaware until June 1985. My office phone number will be (302) 368-5580. I invite you to send information for the spring 1985 CAST Newsletter immediately. Meeting announcements, feature articles, extended abstract of your presentations at AIChE meetings, information on user's groups, messages, opinions, commentaries, polls, advertisements, and so forth are solicited, as are your ideas on novel contributions to the Newsletter and the names of individuals who can do the writing.

CAST Related Papers from San Francisco Meeting

SESSION 8

SINGULARITY THEORY

M. Golubitsky
University of Houston

Paper No. 8a

The strategy of focusing on degenerate bifurcations and then perturbing often helps one find interesting quasi-global behavior. Singularity theory provides methods for implementing this strategy. These methods will be illustrated by discussing two examples: The CSTR and clamped Hodgkin-Huxley equations. These examples illustrate how singularity theory may be applied to bifurcations of both steady states and periodic solutions.

COMPUTER-AIDED APPLIED MATHEMATICS: ANALYSIS OF COMPLEX VISCOUS FREE SURFACE FLOW

K. N. Christodoulou and
L. E. Scriven
University of Minnesota

Paper No. 8b

Linear stability theory and bifurcation analysis are brought to bear by similar computer-aided methods, for which the CRAY-1 and CDC CYBER 205 supercomputers prove cost effective. These methods, lead to a sequence of generalized asymmetric eigenproblems. The paper also exemplifies computer-aided functional analysis of viscous free surface flows.

AN OPERATOR-THEORETIC APPROACH TO LINEAR TRANSPORT PROCESSES IN DILUTE SUSPENSIONS

A. K. Kulshreshtha
and J. M. Caruthers
Purdue University

Paper No. 8c

Dilute suspension theory draws on the solution of boundary value problems formulated on a single particle in the infinite continuous medium. Linear operator--theoretic methods are shown to be a powerful tool in that spectral solutions of associated self--adjoint operators can be obtained for a variety of physically realistic boundary conditions.

BIFURCATION AND STABILITY IN FLAME PROPAGATION

B. J. Matkowsky
Northwestern University

Paper No. 8d

We derive two simplified models from the general equations describing flame propagation. We then describe sequences of bifurcations, and corresponding changes in stability, as parameters of the problem are varied. Such sequences of bifurcations are thought to represent stages in the transition from laminar to turbulent flame propagation.

APPLICATION OF THE THEORY OF GENERALIZED SIMPLE WAVES TO SURFACTANT INJECTION PROCESSES IN POROUS MEDIA

Y. C. Yortsos and S. Saneie
University of So. California

Paper No. 8e

We develop solutions to three--component, two-phase surfactant injection processes in porous media for enhanced recovery of oil. The method of generalized simple waves is to show that concentration and saturation profiles can be obtained with minimal computational requirements for systems following suitable phase equilibria.

VARIATIONAL ANALYSIS OF
CONDUCTION IN TWO-PHASE
RANDOM MEDIA

W. Strieder and D. S. Tsai
University of Notre Dame

Paper No. 8f

Variational methods are considered which bound effective transport properties of random media. Dispersed spheres and randomly oriented fibers were used to model a number of materials of engineering interest. Estimated thermal conductivities of plastic metal composites, fiber glass insulation, and diffusivities of granular and fibrous materials are compared with measured values.

SESSION 27

ON THE USE OF ADAPTIVE
METHODS IN THE SOLUTION
OF COMBUSTION PROBLEMS

M. Smooke
Sandia National Labs.

Paper No. 27a

Efficient numerical solution combustion problems requires that grid points be placed adaptively in the regions in question. We select the points by equidistributing a positive weight function

over consecutive mesh intervals. Both 1D and 2D steady state and transient combustion problems are considered.

ALGORITHMS FOR INTEGRATION
OF COMPLEX REACTION SYSTEMS

C. W. White III
and W. D. Seider
University of Pennsylvania

Paper No. 27b

Strategies to improve efficiency and reliability in the numerical integration of mass and energy balances for a PFTR are evaluated. For combustion reaction systems, modern stiff integrators are very effective. The steady--state, pseudo-steady-state, and chemical equilibrium approximations, and exchanges of independent variables, scaling and arc--length transformations offer little improvement in efficiency and reliability.

SENSITIVITY ANALYSIS OF
SYSTEMS OF DIFFERENTIAL AND
ALGEBRAIC EQUATIONS

M. A. Kramer and J. R. Leis
Massachusetts Inst. of Tech.

Paper No. 27c

Parametric sensitivity equations often arise in dynamic modeling of equilibrium stage processes and solution of partial differential equations. Formulae are developed which can be used to efficiently produce the model sensitivity equations.

DEGREE THEORY AND HOMOTOPY.
TOOLS FOR COMPUTER-AIDED
PROCESS DESIGN

T. L. Wayburn
Clarkson University

Paper No. 27d

This paper presents some of the theory behind homotopy-continuation methods, which have been used recently by some investigators to solve separation problems. Conditions under which these methods are likely to succeed are developed and a few of the difficulties are illustrated by simple examples.

IDENTIFICATION OF SPATIALLY-
VARYING PARAMETERS IN
PARTIAL DIFFERENTIAL
EQUATIONS BY DISCRETE
REGULARIZATION

C. Kravaris
University of Michigan
Ann Arbor, MI
and J. H. Seinfeld
Cal Inst. of Technology

Paper No. 27e

The present work refers to the identification of spatially-varying parameters in partial differential equations. The discrete regularization approach involves the use of the principle of regularization together with an a priori discretization of the unknown parameters via finite-dimensional convergent approximations. Applications to petroleum reservoirs are considered.

A NONLINEAR PROGRAMMING
APPROACH TO DYNAMIC
OPTIMIZATION PROBLEMS

L. T. Biegler
Carnegie-Mellon University

Paper No. 27f

Chemical process problems described by differential-algebraic models are currently optimized by algorithms requiring repeated solution. A simultaneous solution and optimizing strategy that uses orthogonal collocation and an SQP method will be used. Applications to reactor design will be presented.

DYNAMICS OF PERIODICALLY
FORCED CHEMICAL REACTORS

I. G. Kevrekidis
L. D. Schmidt and R. Aris,
University of Minnesota

Paper No. 27g

A method for studying the dynamic behavior of periodically forced chemical reactors is presented. The method yields stability information on harmonic bifurcation, bifurcation to tori and frequency locking, and routes to deterministic chaos.

SESSION 45

A NEW APPROACH TO
BATCH PROCESS DESIGN
--ICI'S BATCHMASTER

G. W. Frank and M. L. Preston
Imperial Chemical Industries PLC

Paper No. 45a

The paper reviews experience and understanding of the requirements of batch process design gained

during the specifications of BatchMASTER, ICI's new batch process flowsheeting system. This system is built on the foundation of ICI's scheduling software, Process Engineering Database developments, and over 15 years' experience with dynamic discrete event simulation language.

TWO CASE STUDIES IN BATCH PLANT DESIGN

S. Ali and M. Malanchini
Istituto Guido Donegani
S. A. Novara, Italy
and T. Ernst

M. Hofmeister and D.W.T. Rippin
Technisch-Chemisches Labor

Paper No. 45b

The application of an academically developed program MULTIBATCH intended for optimization of batch plant design is discussed based on two case studies carried out cooperatively with industry. Difficulties inhibiting the use of such programs for the solution of industrial problems in the batch process area are analyzed and successful remedies outlined.

DETERMINISTIC VARIABILITY ANALYSIS FOR INTERMEDIATE STORAGE IN NONCONTINUOUS PROCESSES

I. A. Karimi
Purdue University

Paper No. 45c

Part 1: Allowability Conditions

Intermediate storage is commonly used to mitigate the effects of process parameter variations in noncontinuous processes. A taxonomy and analysis is presented of the various types of variations. Sufficient conditions are developed which ensure continuity

of periodic operation in the presence of these variations.

Part 2: Storage Sizing for Serial Systems

The allowability conditions of Part 1 are applied to develop intermediate storage sizing expressions for serial systems subjected to process parameter variations. Multiple variations in either starting moments, transfer flow rates or transfer fractions are considered first. These results are then combined using a worst case analysis to develop size estimates under general variations.

SYNTHESIS OF FLEXIBLE HEAT EXCHANGER NETWORKS FOR MULTI-PERIOD OPERATION

C. A. Floudas
Carnegie-Mellon University

Paper No. 45d

Heat exchanger networks in semi-continuous processes must have the flexibility to handle discrete changes in flowrates and temperatures of the process streams. Using as a basis a multiperiod transshipment model, a procedure is proposed to derive network configurations that require minimum utility consumption with the fewest number of heat exchanger units.

APPLICATION OF SIMULATION TO THE CAPACITY PLANNING OF A SPECIALTY CHEMICALS PRODUCTION FACILITY

Richard M. Felder
George B. McLeod, IV
North Carolina State University

Paper No. 45e

A method has been developed to e-

valuate the effects of plant and process modifications on the overall productivity of a multi-product specialty chemicals plant. Simulation studies are first performed on individual processes in each of the production areas in which the processes can be carried out. A linear programming algorithm is then used to determine the maximum improvement in overall plant productivity that can be expected to result from the implementation of any process modification. The results allow management to determine cost-to-benefit ratios of proposed equipment or operating personnel additions before committing any capital to the changes.

SIMULATION OF A LARGE
SCALE MULTIPRODUCT
POLYMER PROCESS USING 'BOSS'

G. Joglekar, CAE Inc.
G. V. Reklaitis
Purdue University

Paper No. 45f

The BOSS flowsheeting system for noncontinuous processes is used to model and study the operation of a large scale multistage, multiunit batch/semicontinuous process involving concurrent production of multiple products. The effects of schedule on utility consumption rates, operator utilization and assignment, and intermediate storage distribution are investigated.

SESSION 63

AN INDUSTRY EVALUATION
OF SPEEDUP

P. K. Gupta & R. C. Lavoie
Exxon Corporation

Paper No. 63a

The paper presents the results of Exxon's evaluation of SPEEDUP, an equation-based process flowsheeting system developed at Imperial College for the steady-state and dynamic modeling of chemical processes. The objectives of the evaluation were to determine whether equation-based systems can be used effectively for steady-state simulation in a commercial environment and to compare SPEEDUP with a commercially proven sequential modular process flowsheeting system.

A STRATEGY FOR PROCESS
ANALYSIS AND DESIGN:
IMPLEMENTATION

Jorge R. Paloschi
Rafiqul Gani
Jose A. Romagnoli
Planta Piloto de
Ingenieria Quimica

Paper No. 63b

The implementation of a strategy for process analysis and design is discussed. This strategy analyzes the operation through studies that relate sensitivity and operability of the process to conditioning of the system of equations representing it. Furthermore, an algorithm is proposed to obtain the initial point for the simulation problem. Applications to practical examples is shown by means of two different types of simulation packages, CHSS and SPEEDUP. One

of the examples consists of a section of an existing ethylene plant.

ANALYSIS OF HETEROGENEOUS
AZEOTROPIC DISTILLATIONS

H. N. Pham and M. R. Doherty
University of Massachusetts

Paper No. 63c

A robust technique for liquid--liquid-vapor equilibrium calculations is able to distinguish between the stable, metastable and unstable regions of a phase diagram. The method has been used to compute residue curve maps for a selection of ternary heterogenous azeotropic mixtures.

THERMODYNAMICALLY
CONSISTENT QUASI-NEWTON
FORMULAE

A. Lucia, D. C. Miller
and A. Kumar
Clarkson University

Paper No. 63d

New quasi-Newton formulae are presented that obey secant conditions and sparsity constraints, while satisfying thermodynamic constraints. Numerical experiments show that these new formulae can result in improved reliability and efficiency.

PARAMETRIC SENSITIVITY
ANALYSIS OF CHEMICAL
PROCESS FLOWSHEETS

M. A. Kramer

Paper No. 63e

Sensitivity analysis aids process design by elucidating the important parameters in a process flowsheet, and by providing statistical information on the sig-

nificance of simulation results. Algorithms for sensitivity analysis of complex flowsheets are presented which are 10 to 100 times more efficient than continuation methods. Both equation-oriented and modular approaches are discussed.

MULTIPLE SOLUTIONS TO
SYSTEMS OF INTERLINKED
DISTILLATION COLUMNS BY
DIFFERENTIAL HOMOTOPY
CONTINUATION

T. L. Wayburn
Clarkson University
J. D. Seader and R. Chavez
University of Utah

Paper No. 63f

This paper describes a computer implementation of homotopy continuation which was used to model two different arrangements of interlinked distillation columns. Using product-purity specifications, so that interlink flow rates were computed rather than specified, multiple solutions were found for both arrangements for a number of reflux ratios.

SESSION-82

DECOMPOSITION ASPECTS IN
THE DESIGN OF MULTIVARIABLE
PROCESS CONTROLLERS

G. Stephanopoulos
Massachusetts Inst. of Tech.
M. Nikolaou
Nat. Tech. University of Athens

Paper No. 82a

The concept of block diagonal dominance has attracted a great deal of attention for the design of multivariable control systems. In this paper, an attempt is made

to elucidate the framework of analysis and interpret these ideas, especially as they pertain to the design of steady state or dynamic controllers.

EVALUATING SIGNIFICANT
ECONOMIC TRADE-OFFS FOR
PROCESS DESIGN AND STEADY-STATE
CONTROL OPTIMIZATION PROBLEMS

W. R. Fisher, M. F. Doherty
and J. M. Douglas
University of Massachusetts

Paper No. 82b

An order-of-magnitude optimization procedure allows rapid screening of flowsheet alternatives. The method exploits the unique characteristics of the chemical process design problem. Quantitative parameters are defined which specify the most important design variables, while preventing the rigor of the optimization from exceeding the accuracy of the economic models used.

OCCURRENCES OF ZEROS IN
OPTIMIZED CHEMICAL PROCESSES

W. J. Schmidt, J. M. Fox and
J. M. Douglas
University of Massachusetts

Paper No. 82c

Steady state optimization of chemical processes results in dynamical system zeros near the origin. One consequence is a lack of control system robustness. This is shown by an example. The phenomenon of input multiplicity is demonstrated.

HIGH PERFORMANCE
MULTIVARIABLE CONTROL
STRATEGIES FOR SYSTEMS
HAVING TIME DELAYS

N. F. Jerome and W. H. Ray
University of Wisconsin

Paper No. 82d

A high performance time delay compensator has been developed which contains the Ogunnaide-Ray (1979) compensator as a special case, reduces to the Smith predictor for a single delay, and approaches the realizable part of the process inverse as a limit. A simple design and implementation procedure is described.

OPERATOR CONTROL THEORY
AND A NEW CLASS OF
NONLINEAR CONTROLLERS

C. G. Economou and M. Morari
Cal. Institute of Tech.

Paper No. 82e

Some strong connections between operator and control theories are established. They motivate a re-examination of the controller design method in the light of iterative operator equation solution procedures. Contraction Principle and Newtonian controllers are developed and their performance and stability characteristics are directly investigated.

QUADRATIC/DYNAMIC
MATRIX CONTROL OF
NONLINEAR CONTROLLERS

C. E. Garcia
Shell Development Company

Paper No. 82f

An application of Shell's QDMC (Quadratic/Dynamic Matrix Control) algorithm has been used to

control a nonlinear process. The method employs differential equations of the system in order to: 1) calculate projected deviations of variables from a specified trajectory; 2) calculate local step response coefficients. Implementation on a semi-batch reactor process is presented.

ON-LINE PARAMETER
ESTIMATION BY SEQUENTIAL
PARTIAL REGRESSION

O. A. Asbjornsen
University of Houston

Paper No. 82g

"Normal regression equations for parameter estimation are solved by standard Gauss eliminations, where the input/residual covariances serve the pivot selection. Parameter updates stop when the improvement in the explanation of the residual becomes insignificant. Practical experience proves the method to be extremely robust. Outlayers indicate dramatic parameter changes."

SESSION 88

SYNTHESIS OF HOMOGENEOUS
AZEOTROPIC DISTILLATIONS

S. G. Levy and M. F. Doherty
University of Massachusetts

Paper No. 88a

An exact algebraic method for calculating minimum reflux ratios in double-feed azeotropic columns has been developed. The resulting procedure allows for a systematic design and synthesis scheme for multi-column azeotropic distillations. Competing entrainers and competing column sequences can be efficiently

screened using this approach.

USE OF COMPLEX COLUMNS
TO ENHANCE HEAT
INTEGRATION OF
DISTILLATION SYSTEMS INTO
TOTAL FLOWSHEETS

E. Hindmarsh, ICI Energy and
Process Synthesis Consultancy

Paper No. 88b

A systems approach and new representation is presented for heat integration of distillation columns into total flowsheets. Process changes are identified for which discrete and reducing utility targets are calculated. The method highlights those complex columns which further enhance heat integration possibilities, as demonstrated by example.

SYNTHESIS OF OPTIMAL
SATURATES SEPARATION
SEQUENCES

D. W. Tedder
Georgia Inst. of Technology

Paper No. 88c

A refinery light ends fractionation problem was studied using a computer optimization program (RUNOPT), dynamic programming, and rank order listing to generate 17 near optimal separation sequences. A total of 23,232 alternative sequences were screened through the evaluation of 437 subproblems. State optimization, tower interactions, and heat exchanger matching were all found to be important. Although the unintegrated rank list of sequences was similar to the ranked list when integration was permitted, sequence shifts were observed. The optimal sequence included heat exchanger

reviewed with particular attention to computer-monitored chemical systems.

PROCESS DYNAMICS AND THE
STOCHASTIC BEHAVIOR OF
BATCH LUMBER KILNS

Ferhan Kayihan
Weyerhaeuser Technology Center

Paper No. 120b

A Monte-Carlo model is developed to predict the moisture content transients of boards during the drying of dimension lumber in batch kilns. Product value depends strongly on the final moisture content distribution which is a function of lumber properties and the drying schedule used. Owing to the inherent property variations, measurement limitations and external process upsets, the same schedule does not yield the best result for every batch. The control policy for this process is defined in terms of an end-point optimal control problem. The paper will discuss the development of the model, the process characteristics and the requirements for the optimal control policy.

DYNAMIC ESTIMATION
OF TEMPERATURE AND
CONCENTRATION PROFILES
FOR CONTROL OF A
PACKED BED REACTOR

L. C. Windes and W. H. Ray
University of Wisconsin
A. Cinar,
Illinois Inst. of Tech.

Paper No. 120c

Effective control and yield maximization of an exothermic packed bed reactor is made possible by estimation of conversion and selectivity from on-line temperature

measurements. A two-dimensional distributed parameter optimal state estimation algorithm is evaluated through simulation and experiments.

OBSERVER DESIGN
BASED ON MODEL
REDUCTION TECHNIQUES

J. E. Gupta, J. C. Vogel
J. A. Porras and J. Romagnoli
Universidad Nacional Del Sur

Paper No. 120d

The use of reduced order dynamic models, based on structural dominance analysis together with filtering techniques, allows the development of an "observer" for efficient control purposes. This approach is applied to an industrial column, and the numerical results thus obtained illustrate its salient features.

COMPARISON OF LINEAR
DISTRIBUTED PARAMETER
FILTERS TO LUMPED
APPROXIMANTS

D. J. Cooper, W. F. Ramirez
and D. E. Clough
University of Colorado

Paper No. 120e

Optimal distributed parameter filters are commonly implemented via an approximating system of lumped Kalman filters. The effect of such an approximation is investigated. The theoretical development shows a loss in spatial correlation for the lumped approximants resulting in slower convergence. This phenomenon is illustrated by two numerical results thus obtained illustrate its salient features.

MODELING EVAPORATOR SYSTEMS
FOR RADIOACTIVE WASTE

Habib Amin, Bechtel Power Corp.
K. C. Chiu, Bechtel Petro., Inc.
David James, Bechtel Power Corp.

Paper No. 120f

A generic computer model is developed for the dynamic simulation of the radioactive waste evaporator systems in nuclear power stations. The developed system component models are integrated with Bechtel's Dynamic Analysis Program to simulate the system's dynamics. The presented example illustrates the strong potential of the model for solving the system's control problems.

EFFECT OF RECYCLE
STRUCTURE ON DISTILLATION
TOWER TIME CONSTANTS

T. J. Mc Avoy and N. Kapoor,
University of Maryland
and T. E. Marlin
Exxon Research and Engineering

Paper No. 120g

Recycle can change the dynamics of a process. Distillation towers are inherently recycle processes. Published time constant estimates of towers can be substantially in error when compared with actual responses. The reason for this is the recycle nature of distillation towers. A greatly improved method of estimating time constants is presented.

SESSION 123

AN ALGORITHM FOR
SCHEDULING PRODUCTION IN
A MULTIPRODUCT SPECIALTY
CHEMICALS PLANT

R. M. Felder and P. M. Kester
North Carolina State University

Paper No. 123a

A procedure has been developed to schedule production for a multiproduct chemical manufacturing facility. The algorithm develops a schedule that minimizes inventory costs while meeting a specified set of product demands. The code has been structured to fit on a microcomputer, to solve fairly large problems, and to be accessible and easy for plant personnel to use. Applications include determining whether product demands can be met with existing plant capacity, calculating the capacity increases needed to meet demands for which present capacity is inadequate, and estimating the impact of shutting down production areas for specified periods of time.

ESSO A.G. CRUDE OIL
SCHEDULING TOOL (CRUST)

I. Suhami
Exxon Corporation

Paper No. 123b

CRUST is an interactive scheduling system, developed for the Supply and Transportation Department of Esso A. G., German affiliate of Exxon. Its purpose is to computerize a large portion of the scheduling and coordination of crude supply for the three German refineries. CRUST allows the scheduler to evaluate

different refinery, pipeline, and ship schedules.

DETERMINATION OF COMPLETION
TIMES FOR SERIAL MULTIPRODUCT
PROCESSES UNDER MIXED INTER-
MEDIATE STORAGE POLICIES

W. Wiede Jr., and G. V. Reklaitis
Purdue University

Paper No. 123c

A recursive scheduling procedure is reported which determines the earliest completion time and intermediate storage assignments for a given product processing sequence on a serial process involving a variety of interstage storage provisions. Any combination of unlimited finite no-intermediate storage or zero-wait processing policies can be accommodated.

APPLICATION OF INTERACTIVE
VISUAL SIMULATION TO
REFINERY OPERATION
SCHEDULING

J. Stewart
Imperial Oil Ltd.

Paper No. 123d

A new computerized system has been developed by Imperial Oil Limited for the scheduling of refinery operations. The program interacts with the scheduler to prepare for crude arrivals, select unit operating conditions, and schedule product blending to meet product demand for up to three months in advance. Volumes and qualities of all products are tracked over time via simplified process and blender models.

The system is micro-computer based, and makes extensive use of interactive computing, simula-

tion. animation and colour graphics.

AN OPERATION PLANNING AND
CONTROLS SYSTEM FOR BATCH
MANUFACTURING

N. Streit
Hewlett-Packard

Paper No. 123e

H-P's Manufacturing Productivity Network for managing information in a manufacturing environment will be described. The system consists of user-customizable, interactive modules for managing materials and production planning and control. A major objective is to facilitate access to inventory and production data from order entry through product shipping.

EQUATION ORIENTED SYSTEM FOR
PRODUCTION SCHEDULING MODELS

P. J. McLellan, G. S. Mueller &
G. R. Sullivan
University of Waterloo

Paper No. 123f

The SPEED-UP equation oriented simulation systems are used for solution of nonlinear refinery processing unit models within a production scheduling framework. For a wide variety of process units, it was found that a mixture of purely equation-based and purely procedural-based approaches yielded convergency properties most suitable for production scheduling systems.

SESSION 131

FEASIBILITY TEST OF A FAULT
DIAGNOSIS ALGORITHM
ON A PILOT PLANT

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Nagatsuta, Yokohama, H. Matsuyama
Hakozaki, Fukuoka, J. Shiozaki
Kyusyu University
Hakozaki, Fukuoka,
and M. Matsushita
Diacel Chem Ind.

Paper No. 131a

A feasibility test of the fault diagnosis algorithm based on the signed digraph was performed on a pilot plant. The plant was composed of two reactors and their peripheral equipment. The effectiveness of adding supplemental measured points in reducing the number of possible candidates to obtain the source of failure was investigated.

ALARM SYSTEMS ALARM ANALYSIS

P. Andow
Loughborough University of Tech.

Paper No. 131b

All modern process plants are equipped with alarm systems. The alarm system often provides the operator with the opportunity to take remedial action prior to trip operation. Alarm systems can be improved by the use of diagnostic aids such as "Alarm Analysis." Alarm analysis can improve operator performance and hence avoid plant shutdowns.

APPLICATION OF EXPERT SYSTEM TECHNIQUES TO FAULT DIAGNOSIS

Ernest J. Henley
University of Houston

Paper No. 131c

In fault-diagnosis applications, IF-THEN production rules organize the expert knowledge regarding fault-isolation. The classifica-

tion of system states can be formulated by:

If [system state i]
& (observable fact)
Then system state

The example provided, has 22 rules for cause-isolation. The interactive conversation informs the operator of:

1. The IF-THEN rule applied.
2. The prerequisite states.
3. A fault-diagnosis.

MODELING OF PROCESS PLANTS FOR RISK AND RELIABILITY

A Shafaghi
Battelle Columbus Laboratories

Paper No. 131d

A method is presented for synthesis of fault trees and an inductive tree for process plants. The method is based on decomposition of the plant into control loop structures. Failure models of the loops are developed and synthesized through their interactions. The plant failure model is used for risk and reliability analysis.

SOLVING TROUBLE SHOOTING PROBLEMS

D. R. Woods
McMaster University

Paper No. 131e

How to solve trouble shooting problems is examined particularly from the viewpoint of training students.