

CACHE NEWS

*NEWS ABOUT COMPUTERS
IN CHEMICAL ENGINEERING
EDUCATION*

No. 39

Fall 1994



**25th Anniversary
Issue**

CACHE NEWS

No. 39

Spring 1994

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THE CACHE CORPORATION

WHAT IS CACHE?

CACHE is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960s the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, fourteen chemical engineering educators met in 1969 to form the CACHE (ComputerAids for Chemical Engineering) Committee. The CACHE Committee was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers including both educators and industrial members and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its ongoing projects. Information on CACHE activities is regularly disseminated through CACHE News, published twice yearly. Individual inquiries should be addressed to:

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CACHE NEWS

The CACHE News is published twice a year and reports news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by D. M. Himmelblau with contributions from a number of CACHE members and representatives.

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Special Message to Chemical Engineering Faculty

By Michael B. Cutlip, University of Connecticut, Outgoing CACHE President

As I complete my two year term as CACHE president, I would like to summarize some of the newer products which can make significant contributions to chemical engineering education. Often in this busy academic environment, we educators do not keep close track of recent educational developments which can be very helpful in our classes. CACHE is marketing several new products which I highly recommend that you consider for educational use with your students.

IBM-Compatible Software by Academic Authors

As more and more students are acquiring their own personal computers, three major products produced by dedicated academics have been made available by CACHE. These programs have inexpensive site licenses allowing for legitimate use on any personal computer at your University. The licenses include use in personal computer labs, on faculty computers, and perhaps most importantly, on student owned computers. The following three products are all continuing to be developed and supported by very committed faculty authors:

- 1) **POLYMATH Numerical Analysis Package** by *Mordechai Shacham of Ben Gurion University in Israel and Mike Cutlip of the University of Connecticut*. POLYMATH is widely used to give students an effective general program which provides most of the standard numerical analysis capabilities in an easy-to-use package. Students can easily and efficiently solve very realistic problems in most of the core chemical engineering subject areas. A significant upgrade of POLYMATH is discussed elsewhere in this newsletter.
- 2) **ChemSep** by *Ross Taylor of Clarkson University*. ChemSep is a suite of programs for performing multicomponent separation process simulations from single stage flash to multistage operations such as distillation, gas absorption and liquid-liquid extraction. Many thermodynamic property models are supported and the program includes a databank for 189 common chemicals.
- 3) **PICLES** by *Doug Cooper of the University of Connecticut*. This Process Identification and Control Lab Simulator is IBM PC compatible software now being used in more than 50 university and industrial

control courses around the world. PICLES is an easy-to-use simulator that provides hands-on experience to those studying this often abstract and mathematical subject. An article about PICLES is also in this newsletter.

NSF/CACHE Software

Three NSF educational grants to Washington, Michigan and Purdue have resulted in exciting and useful new CACHE products:

- 1) **Chemical Reactor Design Toolbox** by *Bruce Finlayson at University of Washington*. This set of computer programs will do simulations of batch or CSTR reactors, plug flow reactors, plug flow reactors with axial dispersion, or 2D reactors with axial dispersion. The program handles mole changes, volume changes, and pressure changes for multiple reactions and heterogeneous reactions. It runs on Unix systems using X-windows
- 2) **Laboratory Experiment Simulators** by *Bob Squires, P. K. Anderson, G. V. Reklaitis, S. Jayakumar, et al. from Purdue University*. A series of six Sun Sparc workstation simulations of industrial processes were designed for the chemical engineering laboratory course, but they can be used in other courses. Emphasis is on planning experiments and analyzing the "experimental" results. Modules are open-ended, and teams of students are typically used. Various industrial companies have supplied realistic problems. Usually a 20 minute video tape is provided for introduction. Conversion is underway to HP, DEC, IBM/RSIC and Silicon Graphics workstations.
- 3) **Michigan Interactive Computer Modules** by *Scott Fogler, Susan Montgomery et al. at the University of Michigan*. Six years of effort have gone into the development of over twenty four interactive computer modules designed to enhance the teaching of chemical engineering courses in material and energy balances, fluids and transport, separations, and reactor design. These highly interactive modules utilize the computational and graphical animation capabilities of IBM compatible personal computers.

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CACHE 25th Anniversary Activities at the San Francisco AIChE Meeting

Session 183 - Special Symposium
"Computers in Chemical Engineering Education - 25 Years of CACHE"
CACHE 25th Anniversary Reception

The upcoming AIChE meeting will mark the celebration of CACHE's 25th year anniversary. The special events are open to everyone so please plan to attend.

The session on "Computers in Chemical Engineering Education - 25 Years of CACHE" will provide current overviews and futuristic extrapolations in various areas of Chemical Engineering with presentations by prominent educators. The schedule will be as follows:

Wednesday, November 16th, 1:00 PM
Grand Ballroom A - San Francisco Hilton
Hotel

- | | |
|---------|---|
| 1:00 PM | Introduction
by Michael B. Cutlip, University of Connecticut, Storrs, CT |
| 1:05 PM | Process Control Education: Present, Past, Future
Paper No. 183a by Thomas F. Edgar, University of Texas, Austin, TX |
| 2:00 PM | Ghosts of Interactive Computing: Past, Present and Future
Paper No. 183b by H. Scott. Fogler, University of Michigan, Ann Arbor, MI |
| 2:50 PM | Coffee Break |
| 3:10 PM | Knowledge, Computers, and Process Engineering: A Critical Synthesis
Paper No. 183c by George Stephanopoulos, Massachusetts Institute of Technology, Cambridge, MA |
| 4:00 PM | 2001 - A Computing Odyssey
Paper No. 183d by Brice Carnahan, University of Michigan, Ann Arbor, MI |
| 4:50 PM | Concluding Remarks
by David M. Himmelblau, University of Texas, Austin, TX |

CACHE 25th Anniversary Reception
Wednesday November 16th, 6:00 PM
Continental Ballroom 4 - San Francisco Hilton

Everyone is invited to attend the special activities and demonstrations at the reception which will start promptly at 6:00 PM in the Continental Ballroom 4 of the San Francisco Hilton. The activities will include:

Introductions and CACHE Accomplishments Highlights - by host Gintaras (Rex) V. Reklaitis, Purdue University, West Lafayette, IN

The CACHE CD-ROM - A Short Overview - by Editor Peter R. Rony, Virginia Polytechnic & State University, Blacksburg, VA

Special Note - All academic and industrial chemical engineers who attend the CACHE Reception will get a free copy of the CACHE CD-ROM. This will be a valuable personal resource for many years and will eventually be a collector's item. It will include a single user license for most of the CACHE current products including CHEMSEP, PICLES, POLYMATH, University of Michigan Educational Modules, associated manuals plus much, much more. More details are included in the CD-ROM article by Peter Rony. Free copies are available only to those attending the reception who sign up on the distribution sheet upon receiving the CD-ROM.

CACHE 25 Anniversary Monograph - Content Overview - by Editor Brice Carnahan, University of Michigan, Ann Arbor, MI

Special Note - Special priced Monograph orders will be taken from those attending the reception.

Displays and Demonstrations of Current CACHE Products - CACHE task forces and committees will be displaying and/or demonstrating the latest in educational materials. CACHE publications will be on display.

CACHE Memorabilia Display from the last 25 Years - Interesting items from the past will be on display from those associated with CACHE over the years.

Sumptuous Hors D'oeuvres and Liquid Refreshments
The reception will continue until about 8 PM.

Abstracts for the CACHE Special Session "Computers in Chemical Engineering Education - 25 Years of CACHE"

1994 AIChE Meeting in San Francisco
Session 183 on Wednesday, November 16th
Grand Ballroom A - San Francisco Hilton Hotel

Process Control Education: Past, Present, and Future (1:05 PM)

By Thomas F. Edgar, University of Texas

The practice of chemical process control has undergone significant changes since the 1970s when distributed computer control systems were first introduced. These changes have appeared in the process industries in several overlapping periods, each demanding an increased level of sophistication in process control:

- (1) introduction of computer control
- (2) energy conservation
- (3) safety and environment
- (4) quality control/international competition
- (5) multivariable optimizing control

Each of these periods has increased the breadth of technology that entry-level engineers must understand, although the content of the typical undergraduate course in process control has not changed much during the past 20 years. This is because the standard undergraduate course focuses mainly on dynamic systems and design of single loop feedback controllers, topics which do not necessarily intersect with the subjects mentioned above. On the other hand, advanced control algorithms, such as feedforward, supervisory, multivariable, and adaptive control, are now routinely employed to maintain plant operation close to the economic optimum. In addition, a comprehensive course in process control could cover other topics such as:

- alarms, safety systems
- expert systems
- computer control hardware
- dynamic simulation
- unit operations control

- batch process control
- statistical process control
- data reconciliation
- real-time computing
- state space analysis
- effect of process design on control
- model identification
- plant control strategies, case studies
- discrete-time systems

The content of a typical undergraduate process control course is not intended to train process control specialists. Rather it presents the key concepts in dynamics and control and attempts to inculcate in B.S. chemical engineers an understanding of transient operations and the influence of feedback control on responses.

Most undergraduate courses have the following learning objectives:

- *Understanding the difference between dynamic and steady state behavior.* Courses in chemical engineering generally deal with steady state analysis only. This fact sets apart the subject matter in process control from other courses in the curriculum. Mathematical modeling is a key ingredient.
- *Becoming proficient in analysis of dynamic systems.* The principal tool employed is Laplace transforms. As long as the course focus is on linear continuous systems, Laplace transforms will always be the starting point, unless this is covered in a prior course in mathematics. The amount of emphasis on Laplace transform operations may be diminishing due to the availability of commercial software.
- *Learning the effect of feedback control and several industrially-accepted methods of tuning PID controllers.* This leads to the issues of stability, performance, and robustness in designing feedback controllers. Computer simulation with interactive graphics is a key pedagogical tool, also based on professional software.

- *Appreciating the benefits of advanced methods such as feedforward and cascade control.* Students should know under what conditions various methods should be implemented.
- *Exposure to modern instrumentation and controller hardware as practiced in industry.* In particular, a digital control system interfaced to an actual process should be included in the control course or as part of a unit operations laboratory.

Table 1 shows the typical course content for a 15-week process control course based on current textbooks.

Table 1
Course Outline for Process Control (ca. 1994)

1. Introductory concepts: feedback vs. feedforward control (1 week)
2. Mathematical modeling of physical systems (1 week)
3. Linear system analysis: Laplace transforms (2 weeks)
4. Response characteristics of typical process systems (1 week)
5. Controller hardware, instrumentation (1 week)
6. Closed-loop analysis, stability calculations (1 week)
7. Tuning of PID controllers (2 weeks)
8. Frequency response analysis (1-2 weeks)
9. Advanced control methods: feedforward, cascade, multivariable, adaptive, supervisory, etc (3-4 weeks)
10. Plant control strategies, case studies (1 week)
11. Miscellaneous topics

The above outline excludes time spent in an associated process control laboratory.

The task of covering the basic material as well as advanced topics in a 15 week course is indeed herculean; there is a need to streamline the existing courses and de-emphasize certain topics. The recent availability of professional software such as MATLAB offers capabilities in simulation and controller tuning that simply were not available ten years ago. This software can also be linked to dynamic simulations of physical models in order to show the impact of nonlinear, multivariable behavior. While satisfactory software implementations of such simulators are not universally available, there has been considerable progress in this area. With the software currently available, it is not clear why several weeks of class time must be devoted to the intricacies of Laplace transform manipulations.

What will the state of affairs in process control be in the year 2000? While most educators believe the

undergraduate students of that era will be more facile with the use of computers, it is unlikely that there will be a quantum jump in the mathematical preparation of those students. So the starting point of a typical course will be about the same as it is now. However, the industrial environment where process control is carried out will probably be quite different than it is today. Because of greater integration of the plant equipment, tighter quality specification, and more emphasis on maximum profitability while maintaining safe operating conditions, the importance of process modeling and control will continue to increase. Very sophisticated computer-based tools will be at the disposal of plant personnel, who will at least need to understand the functional logic of such devices. Controllers will be self-tuning, operating conditions will be optimized frequently, total plant control will be implemented using a hierarchical (distributed) multivariable strategy, and expert systems will help the plant engineer make intelligent decisions (those he or she can be trusted to make). Plant data will be analyzed continuously, reconciled using material and energy balances with optimization, and unmeasured variables will be reconstructed using parameter estimation techniques.

How much emphasis needs to be placed on advanced techniques in the year 2000 course? Should we abandon analog (continuous) analysis methods in favor of digital ones such as z-transforms? What about the PID controller? Will it be replaced by a more general approach based on nonlinear programming? The answers to these questions are complicated. In the year 2000, there will probably be sufficient computing capability available in each process plant (via distributed control) to implement any or all advanced techniques. There may still be single-loop panel-based controllers and control systems utilizing personal computers; while these can communicate with higher level computers, they will employ many different algorithms and functions than those offered in the standard PID controller today. By then the standard undergraduate control course can emphasize discrete-time control. Laplace transforms could be eschewed in favor of discrete time analysis (difference equations) but not necessarily z-transforms. Laplace transforms and linear dynamic systems could be (appropriately) taught in the mathematics department. The selection of topics will require a reasonable level of training in fields such as optimization. In the future we may use nonlinear programming tools in the same way as we employ numerical analysis for simulation today. The student does not need a deep understanding of the numerical details involved in order to have confidence in the answers. Optimization can also provide a unified approach for model identification and parameter estimation.

Ghosts of Interactive Computing: Past, Present, and Future (2:00 PM)

By H. Scott Fogler, University of Michigan

Interactive Computer Experiments and Simulations

Kulik and Kulik reported that most studies found that computer-based instruction had positive effects on students. Specifically, students:

- learn more,
- learn faster, (average reduction in instructional time in 23 studies was 32%),
- like classes more when they received computer help,
- develop more positive attitudes toward computers when they receive help from them in school.

By focusing energy on interactive computing, these positive effects can be realized. Consequently we are developing interactive computing modules that have an open-ended decision-making component that allows the students to practice their divergent thinking skills. Interactive computing modules will help the students' development of divergent thinking skills by providing exercises with a wide number of branch points. At each point the students must make a decision as to which path to follow to the next branch point. Here the students get practice at making decisions in gray areas and also are provided with a multitude of solutions because of all the branching. One example we have developed to illustrate this technique is the design of experiments and collection of data to synthesize a rate law.

Interactive computing simulations provide another way for students to gain experience in making decisions in gray areas and in solving open-ended problems. We shall refer to these interactive exercises and simulations as modules. These interactive computer modules can provide a students with a variety of problem definition alternatives and solution pathways to follow, thereby exercising their divergent-thinking skills. Modules can also provide for the planning of experiments by allowing the students to choose experimental systems, to take simulated "real" data, to modify experiments to obtain data in different parameter ranges, to manipulate data so as to discriminate among mechanisms, and to design a piece of equipment of process. We have already demonstrated that IBM PC simulations possess these pedagogical features.

One of the first major products of CACHE Corporation was the computer programs developed in the late 1960s on punch cards for the core courses in chemical engineering. About this same time, the first use of interactive computing in education was being developed in the Chemistry department at the University of Illinois using the PLATO (Programmed Logic for Automatic Teaching Operations) system. With the PLATO system each terminal had a television screen and a keyboard that the students used to carry out their self paced instructional lessons. While the first interactive lessons used Yes/No and Key word responses (e.g. does the unknown react with C_6H_5COCl in pyridine?). Later lessons simulated actual laboratory experiments. For example the students explored the reaction of an olefin with bromine in methanol by varying the initial concentrations. Using known kinetic data the computer immediately calculates and displays the product composition. By experimenting with several sets of reaction conditions the students understanding of the completion involved in the reaction. Other lessons included the construction of a NMR spectra, synthesis pathways, and determination of the unknowns.

What We Have Learned

A significant portion of our efforts has gone to the development of a pedagogical philosophy that makes use of the computer's graphic, interactive, and computational capabilities. In addition, the sophistication required to satisfy a more computer-oriented student body has resulted in the need for more "polished" modules that in the past. The resulting interactive computer module should be a learning experience that supplements the typical classroom and standard homework activities.

Table 1
Consideration in Developing Computer Modules

- Ease of use
- Introduction of new technologies
- Maintaining the focus on the concepts
- No tediousness!
- Promoting learning
- Individual guidance

There are many advantages to using computer-based learning tools. There are also some pitfalls that one must be aware of and avoid. In addition to ensuring the technical accuracy of the material and simulations in the

- *Appreciating the benefits of advanced methods such as feedforward and cascade control.* Students should know under what conditions various methods should be implemented.
- *Exposure to modern instrumentation and controller hardware as practiced in industry.* In particular, a digital control system interfaced to an actual process should be included in the control course or as part of a unit operations laboratory.

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What will the state of affairs in process control be in the year 2000? While most educators believe the

undergraduate students of that era will be more facile with the use of computers, it is unlikely that there will be a quantum jump in the mathematical preparation of those students. So the starting point of a typical course will be about the same as it is now. However, the industrial environment where process control is carried out will probably be quite different than it is today. Because of greater integration of the plant equipment, tighter quality specification, and more emphasis on maximum profitability while maintaining safe operating conditions, the importance of process modeling and control will continue to increase. Very sophisticated computer-based tools will be at the disposal of plant personnel, who will at least need to understand the functional logic of such devices. Controllers will be self-tuning, operating conditions will be optimized frequently, total plant control will be implemented using a hierarchical (distributed) multivariable strategy, and expert systems will help the plant engineer make intelligent decisions (those he or she can be trusted to make). Plant data will be analyzed continuously, reconciled using material and energy balances with optimization, and unmeasured variables will be reconstructed using parameter estimation techniques.

How much emphasis needs to be placed on advanced techniques in the year 2000 course? Should we abandon analog (continuous) analysis methods in favor of digital ones such as z-transforms? What about the PID controller? Will it be replaced by a more general approach based on nonlinear programming? The answers to these questions are complicated. In the year 2000, there will probably be sufficient computing capability available in each process plant (via distributed control) to implement any or all advanced techniques. There may still be single-loop panel-based controllers and control systems utilizing personal computers; while these can communicate with higher level computers, they will employ many different algorithms and functions than those offered in the standard PID controller today. By then the standard undergraduate control course can emphasize discrete-time control. Laplace transforms could be eschewed in favor of discrete time analysis (difference equations) but not necessarily z-transforms. Laplace transforms and linear dynamic systems could be (appropriately) taught in the mathematics department. The selection of topics will require a reasonable level of training in fields such as optimization. In the future we may use nonlinear programming tools in the same way as we employ numerical analysis for simulation today. The student does not need a deep understanding of the numerical details involved in order to have confidence in the answers. Optimization can also provide a unified approach for model identification and parameter estimation.

Ghosts of Interactive Computing: Past, Present, and Future (2:00 PM)

By H. Scott Fogler, University of Michigan

Interactive Computer Experiments and Simulations

Kulik and Kulik reported that most studies found that computer-based instruction had positive effects on students. Specifically, students:

- learn more,
- learn faster, (average reduction in instructional time in 23 studies was 32%),
- like classes more when they received computer help,
- develop more positive attitudes toward computers when they receive help from them in school.

By focusing energy on interactive computing, these positive effects can be realized. Consequently we are developing interactive computing modules that have an open-ended decision-making component that allows the students to practice their divergent thinking skills. Interactive computing modules will help the students' development of divergent thinking skills by providing exercises with a wide number of branch points. At each point the students must make a decision as to which path to follow to the next branch point. Here the students get practice at making decisions in gray areas and also are provided with a multitude of solutions because of all the branching. One example we have developed to illustrate this technique is the design of experiments and collection of data to synthesize a rate law.

Interactive computing simulations provide another way for students to gain experience in making decisions in gray areas and in solving open-ended problems. We shall refer to these interactive exercises and simulations as modules. These interactive computer modules can provide a students with a variety of problem definition alternatives and solution pathways to follow, thereby exercising their divergent-thinking skills. Modules can also provide for the planning of experiments by allowing the students to choose experimental systems, to take simulated "real" data, to modify experiments to obtain data in different parameter ranges, to manipulate data so as to discriminate among mechanisms, and to design a piece of equipment of process. We have already demonstrated that IBM PC simulations possess these pedagogical features.

One of the first major products of CACHE Corporation was the computer programs developed in the late 1960s on punch cards for the core courses in chemical engineering. About this same time, the first use of interactive computing in education was being developed in the Chemistry department at the University of Illinois using the PLATO (Programmed Logic for Automatic Teaching Operations) system. With the PLATO system each terminal had a television screen and a keyboard that the students used to carry out their self paced instructional lessons. While the first interactive lessons used Yes/No and Key word responses (e.g. does the unknown react with C₆H₅COCl in pyridine?). Later lessons simulated actual laboratory experiments. For example the students explored the reaction of a olefin with bromine in methanol by varying the initial concentrations. Using known kinetic data the computer immediately calculates and displays the product composition. By experimenting with several sets of reaction conditions the students understanding of the completion involved in the reaction. Other lessons included the construction of a NMR spectra, synthesis pathways, and determination of the unknowns.

What We Have Learned

A significant portion of our efforts has gone to the development of a pedagogical philosophy that makes use of the computer's graphic, interactive, and computational capabilities. In addition, the sophistication required to satisfy a more computer-oriented student body has resulted in the need for more "polished" modules that in the past. The resulting interactive computer module should be a learning experience that supplements the typical classroom and standard homework activities.

Table 1
Consideration in Developing Computer Modules

- Ease of use
 - Introduction of new technologies
 - Maintaining the focus on the concepts
 - No tediousness!
 - Promoting learning
 - Individual guidance
-

There are many advantages to using computer-based learning tools. There are also some pitfalls that one must be aware of and avoid. In addition to ensuring the technical accuracy of the material and simulations in the

module, there are other considerations we have come aware of through our testing and the comments of the external faculty testers. Some of the aspects of the use of interactive computer modules in engineering education that should be considered by all computer module developers are summarized in Table 1.

We have come a long way since that time as current products used in core courses include Interactive Computer Modules, POLYMATH, and Pickles.

Project History

In the early 1970s the authors developed a number of modules on reaction engineering for use on the University of Michigan's mainframe time-sharing computer. When these simulations were demonstrated at the national meeting, they were enthusiastically received by chemical engineering faculty at other colleges and universities, several of whom requested copies of the programs. Unfortunately, these interactive programs were not easily transportable to computing environments at other universities. In particular, idiosyncrasies in the local graphics-display software caused much of the transportability problem, although operating-system incompatibilities also played a role. However, in response to the rapid evolution of microcomputer-based work stations, many universities have undertaken major microcomputer acquisitions for their students, and today, students in virtually every chemical engineering department in the U.S. and Canada have access to a large number of IBM (or IBM-compatible) personal computers. In the early 1980s, many of the original reaction engineering modules were translated to an IBM format, using BASICA.

Table 2
Primary Components of Interactive Computer Modules

- Introduction
- Review of pertinent fundamentals
- Demonstration
- Interactive exercises
- A branching component
- A solution to the exercise
- Evaluation

In the not too distant future, multimedia modules with video clips, interactive computer textbooks, and virtual reality will be used in chemical engineering

courses. This presentation will discuss effective and innovative uses of current CACHE products in the classroom along with the future of interactive computing (e.g. virtual reality) in graduate and undergraduate chemical engineering education.

References

Kulik, C. C. and J. A. Kulik, *AEDS Journal*, 19, p. 81, (1986).

Kulik, J. A. and C. C. Kulik, *Contemporary Education Psychology*, 12, p.222, (1987).

Knowledge, Computers, and Process Engineering: A Critical Synthesis (3:10 PM)

*By George Stephanopoulos
Massachusetts Institute of Technology*

Computers have become a pervasive presence in every aspect of process engineering activities. From product formulation, through process definition and development, process design and engineering, to process operations and control, computer-based engineering methodologies and computer technology (software and hardware) are shaping almost everything we do, as well as how we organize ourselves and our teams to do it.

In the growing pervasiveness of the computer's presence it is important to step back for a while and take a critical view of how computers are used and abused in process engineering and how the explosive progress of hardware and software technology is shaping and distorting our views of automation. Central in this critical review is the role of knowledge (or lack of it) and its use in computer-aided process engineering. Numerical algorithms, databases, expert and fuzzy systems, neural networks and neural controllers, planners-schedulers, graphic user interfaces, etc. etc., are all different manifestations of the same core intention: harvest, express, and utilize all forms of knowledge in automating an increasingly broadening set of process engineering activities.

In this paper, we will discuss how modern computer science and technology is defining how to extract, articulate, and automate the use of all available knowledge. We will see how the fragmentation, uncertainty, and sources of knowledge are affecting process engineering methodologies and their computer-aided implementation. Finally, we will attempt a synthesis and outline a synergistic evolution of knowledge-computers in future process engineering.

2001 - A Computing Odyssey (4:00 PM)

By Brice Carnahan, University of Michigan

In 1945, Vannevar Bush predicted development of the Memex, a device with strong resemblance to the personal computer:

... for individual use, about the size of a desk, with display and a keyboard that would allow quick reference to private records, journal articles, newspapers, and perform calculations."

In 1967, Vannevar Bush wrote:

Will we soon have a personal machine for our own use? Unfortunately not!"

These two quotes from one of the preeminent researchers/seers in the early history of electronic computing show how remarkably right and just as remarkably wrong predictions about the future of computing can be.

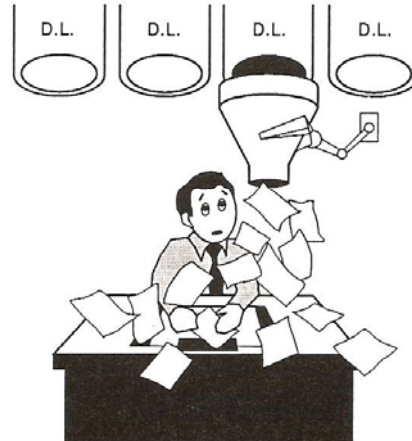
Most new technologies follow the traditional S-shaped curve for innovation and growth that ends with an asymptotic approach to maturity. Fifty years after the ENIAC, we find that by almost any measure (processor speed, hardware architecture, display capability, communication rate, software power, ease of use, model complexity, gross economic activity), "computing" is still in the acceleration phase of its S curve (if it has one).

One long-term prediction is almost certain to be true; the future will be a digital one. However, detailed projections stretching beyond ten years or so are almost certain to be more wrong than right. Hence, Kubrick's 2001 of the title; seven years from the present and one year beyond the millennium, 2001 seems an appropriate target date for looking ahead.

The author will attempt to assess recent developments and current trends, and to make some predictions about the computing scene (particularly the educational computing scene) in 2001.



Electronic mail overload



Conventional filtering

Communications of the ACM

The 25th Anniversary CACHE CD-ROM

By Peter R. Rony, Virginia Tech, CACHE ad hoc Task Force on CD-ROM Technology

Introduction

In our March 19, 1994, CACHE News (Spring 1994), and CAST Communications (Winter 1994) announcements we stated that the 25th-Anniversary CACHE CD-ROM is a single CD-ROM disc whose objectives are:

- (1) to demonstrate new computer technology (e.g., images, audio, video, animation, visualization, sequential presentations, multimedia presentations, visual data analysis) useful in chemical engineering education; and
- (2) to provide a set of software "deliverables" to the target audience — ChE students and faculty — for the CD-ROM.

Adobe Acrobat Reader on the 25th-Anniversary CACHE CD-ROM

The editor has used Adobe Acrobat software — Exchange, Distiller, and Reader — on Windows, Macintosh, and DOS platforms extensively since the introduction of the product in June 1993. Adobe Systems, Inc., as reported in CAST Communications (Winter 1994) and CACHE News (Spring 1994), promotes Adobe Acrobat technology through the Adobe Acrobat (TM) User Group program. CACHE Corporation is now an official Adobe Acrobat User Group, which permits CACHE to distribute copies of Acrobat Reader for DOS, Windows, and Macintosh platforms to all of its CACHE-member departments and faculty, approximately 150 chemical engineering departments (see CACHE News, Spring 1994 listing) and perhaps as many as 2000 CACHE-member chemical engineering faculty and interested students. Two or three versions of Acrobat Reader will be on the 25th-Anniversary CACHE CD-ROM disc, perhaps in two forms: (1) as executable Windows and Macintosh versions of Acrobat Reader (Windows will be used in preference to DOS), and (2) as installable DOS, Windows, and Macintosh versions of Acrobat Reader (in a manner similar to the way they appeared on the 1993 Adobe Systems, Inc. Annual Report CD-ROM).

Acrobat Reader is being provided at no cost to CACHE-member departments, faculty, and students as a "deliverable" of the CACHE ad hoc task force on CD-ROM Technology. By becoming an Adobe Systems

Acrobat User Group and by disseminating Acrobat Reader in the manner stated above, CACHE hopes to encourage the use of Acrobat technology as one possible standard for electronic document viewing within chemical engineering. Adobe Systems, Inc. promises exciting improvements in their version 2.0 of Adobe Acrobat, which the editor has seen as a beta tester.

Authoring Software and Computer Platforms

Three candidates for authoring software for the CACHE CD-ROM were considered:

- (1) Macromedia, Inc. (TM) Authorware 2.01,
 - (2) Asymetrix Corporation (TM) Multimedia ToolBook (TM) 3.0, and
 - (3) Microsoft Corporation Multimedia Viewer (TM) 1.0.
- The editor selected Authorware 2.01 as the primary authoring software because it was available for both Windows and Macintosh platforms. An additional, and important, factor in the editor's choice of Authorware was the fact that Virginia Tech has a site license, available to all students and faculty, for Authorware. Without the site license, Authorware software would have been too expensive, and either Multimedia ToolBook or Multimedia Viewer would have been selected.

Authorware version 2.01 was employed. The majority of the Authorware GUI programming was performed using Authorware for Windows 2.01 (APW). A smaller CACHE CD-ROM GUI using Authorware for Macintosh (APW) will not be created, as originally proposed, because of time limitations and the limited number of Macintosh files submitted. Demos of Multimedia Toolbook version 3.0 may be included on the CACHE CD-ROM, depending upon whether or not they can be used with a runtime version.

"Launching" Adobe Acrobat Reader from an Authorware GUI

Adobe Acrobat Reader for Windows, installed on a CD-R (write-once) disc, works flawlessly when "launched" (executed) from an Authorware GUI program using the JumpOutReturn() command. This is a significant result for all documentation (e.g., Phillips Petroleum lectures, software manuals) that will appear on the 25th-Anniversary CACHE CD-ROM.

"Launching" Windows 3.1 Executables from an Authorware GUI

As with the case with Acrobat Reader for Windows, all Windows 3.1 executable programs work well when launched from an Authorware GUI program using the `JumpOutReturn()` command.

"Launching" DOS Executables from an Authorware GUI

Launching DOS executable (*.EXE) files from an Authorware GUI program using the `JumpOutReturn()` command is not always reliable. One program, it was discovered, cannot be executed when launched from within Windows 3.1 even when a *.PIF file exists. Another program failed to execute from any write-only disc — e.g., a write-protected 1.44-inch floppy disc, a CD-R disc, or a write-protected 128 MB magneto-optical disc. The most successful, consistent approach to launching DOS executables was through the execution of *.PIF files.

Electronic Images and Icons

Colorful bitmap (*.BMP, *.PCX, *.GIF, etc.) images and icons were solicited to spruce up the appearance of the Authorware displays. Click-touch regions and buttons were tested, but abandoned in favor of gray Authorware push buttons. A vigorous attempt was made to obtain appropriate corporate and university logos, images that depicted the purpose of demonstration software, etc. Contributors are thanked for the extra time they spent on acquiring their respective logos.

Multimedia Contributions

If one would define the genre of multimedia to include either digital audio, digital video, or digital animation, then so far there exists few multimedia programs from academia on the September 19, 1994 draft version of the 25th-Anniversary CACHE CD-ROM. The downside to multimedia programs is that they consume substantial memory. The upside is that multimedia educational software represents one software future for chemical engineering education.

Chemical Engineering Department Contributions

Few departments responded to the Call for Contributions to the CACHE CD-ROM. Copy for the "Call for Contributions" — which contained the May 1, 1994 deadline for submission of intention to contribute — was submitted to CACHE News during February

1994, but the Spring 1994 issue did not reach CACHE-member faculty until late April 1994, shortly before the deadline.

The Authorware CACHE CD-ROM Graphical User Interface (GUI)

One month was spent during summer 1994 developing the basic structure of a graphical user interface (GUI) for the 25th-Anniversary CACHE CD-ROM. The task confronting the editor of the CD-ROM was that the GUI was not for the typical Authorware courseware project — namely, an interactive, computer dialog between faculty member and student. Rather, the GUI provided an organizing metaphor for a "heterogeneous" CD-ROM consisting of multi-platform executable and document files from a variety of sources — chemical engineering departments, chemical engineering faculty, student projects, industrial organizations, professional organizations, and so forth.

The CACHE CD-ROM editor spent two-thirds of the summer: (a) testing the ability of authoring software to accomplish two critical objectives for the CD-ROM, namely, to launch executable programs and to launch documents and manuals using Acrobat Reader; (b) acquiring files from CACHE, academic, and industrial software organizations; (c) selecting a corporate sponsor for the CACHE CD-ROM; and (d) polishing and refining the authoring software, which will provide the basic graphical user interface (GUI) for the CACHE CD-ROM.

Currently, the GUI metaphor being used is the Authorware "perpetual-response-menus" approach, as described in excellent detail on pages 5-143 to 5-158 of the "Authorware 1.0 Reference" manual. Simply stated, the following tentative categories appear on a Windows 3.1 menu bar located at the top of the CRT screen: Files, Install, Tutorials, CACHE, Depts, Software, AICHe, Phillips1, Phillips2, and Internet; these categories are still in flux as of September 19, 1994, the day this report is being revised. The current contents of these categories include the following menu items:

Files — Start Over; Exit Install — Read This First; Authorware GUI; How to Use Menus; Important Hints; Copyrights; etc. CACHE — POLYMATH, PICLES, DIGEST, CHEMSEP, CACHE Catalog Depts — Michigan, LSU, Arizona State, Brigham Young, Wisconsin, Colorado State, Queen's University, University of Capetown Software — SimSci, AspenTech, Heat Transfer Research Institute, Adobe Systems, Autodesk (?), Macromedia, Asymetrix, Molecular Design Ltd., Keith Phillips — All Phillips Petroleum lectures at Oklahoma State University since 1967 Internet — Trumpet Winsock, Mosaic, HGopher, Trumpet, WS_FTP, QWS3270, and others.

The attractive feature of the perpetual-response-menus capability is that any of the above nine menu categories can be accessed "perpetually" at any point during a running Authorware GUI program. The editor felt that such ready access was superior to a nested sequence of push-button screens. The downside aspect of the perpetual response menus is that the access time to any given menu item is increased (the search process for the menu categories and items requires time that depends upon the number of categories and items present).

When Will the 25th-Anniversary CACHE CD-ROM be Distributed?

The 25th Anniversary CACHE CD-ROM is scheduled for distribution at the San Francisco AIChE annual meeting during November 13-18, 1994. Up to two copies of the CD-ROM disc will be distributed to each CACHE-member department, one to the department and a second to the local AIChE student chapter, if it exists. Perhaps one of these two copies could be presented to the CD-ROM collection at the university library. It is also planned to distribute free copies to students who attend the AIChE student chapter breakfast at the San Francisco AIChE meeting.

In Summary...

As of September 19, 1994, the CACHE CD-ROM is on schedule. Most contributions are in hand, or are stated by their contributors to be forthcoming. The basic characteristics of the Authorware for Windows GUI have been selected, and both (a) addition of contributions and (b) polishing of the GUI are in progress. A draft CD-R will be sent for testing by several CACHE trustees during late September or early October 1994.



Why, a four-year-old child could understand this.
Someone get me a four-year old child. (Goucho Marx)



Four to six weeks in the lab can save you an
hour in the library. (G.C. Quadererer)

CACHE 25th Anniversary Monograph

By Brice Carnahan, University of Michigan

As part of its 25th Anniversary celebration, CACHE is preparing a Monograph entitled *Past, Present, and Future of Computing in Chemical Engineering Education*. The individual chapter titles and contributing authors are shown below. Brice Carnahan is serving as editor. Currently available chapters will appear as Acrobat-readable files on the CACHE 25th Anniversary CD-ROM (to be distributed at the AIChE meeting in November) which is being prepared by Peter Rony (Virginia Tech.). A copy of the complete printed volume will be distributed to every Chemical Engineering faculty member early in 1995.

1. History of CACHE and its evolution
J. D. Seader (University of Utah)
2. History of computing in chemical engineering education
B. Carnahan (University of Michigan)
3. Role and impact of computers in education
R. Mah (Northwestern University)
D. Himmelblau (University of Texas)
4. Computing skills in the chemical engineering curriculum
T. Edgar (University of Texas)
J. Kantor (University of Notre Dame)
5. Interactive computer-aided instruction
S. Fogler (University of Michigan)
S. Montgomery (University of Michigan)
6. Equation solving and data correlation
M. Shacham (Ben Gurion University)
M. Cutlip (University of Connecticut)
N. Brehner (Tel-Aviv University)
7. Thermodynamics and property databases
A. Fredenslund (Tech. University Denmark)
G. Kontogeorgis (Tech. University Denmark)
R. Gani (Tech. University Denmark)
8. Reaction engineering
S. Fogler (University of Michigan)
9. Transport phenomena
B. Finlayson (University of Washington)
A. Hrymak (McMaster University)
10. Separations Processes
R. Taylor (Clarkson University)
11. Conceptual design and process synthesis
J. Douglas (University of Massachusetts)
J. Sirola (Eastman Chemical Co.)
12. Process simulation
L. Biegler Carnegie-Mellon University
J. D. Seader (University of Utah)
W. Seider (University of Pennsylvania)
E. Rosen (Monsanto Co.)
13. Optimization
I. Grossmann (Carnegie-Mellon University)
14. Design case studies
I. Grossmann (Carnegie-Mellon University)
M. Morari (California Inst. of Tech.)
15. Process control
Y. Arkun (Georgia Inst. of Tech.)
C. Garcia (Shell Oil Co.)
16. Laboratory automation
J. Wright (Canadian Paper Research Inst.)
D. Mellichamp (University of California Santa Barbara)
B. Joseph (Washington University)
17. Computer communications
P. Rony (Virginia Polytechnic Inst.)
18. Intelligent systems
G. Stephanopoulos (Massachusetts Inst. Tech.)
J. Davis (Ohio State University)
V. Venkatasubramanian (Purdue University)
19. Programming Paradigms
G. Stephanopoulos (Massachusetts Inst. Tech.)
20. Visualization
A. Hrymak (McMaster University)
21. Evolution of computer hardware
S. Kim (University of Wisconsin)
22. Future directions
G. Reklaitis (Purdue University)
J. Sirola (Eastman Chemical Co.)

Teaching Computer-Aided Biochemical Process Design Based on BioPro Designer

by Vital Aelion and Demetri Petrides, New Jersey Institute of Technology

Introduction

Teaching biochemical process design, either at the undergraduate or at the graduate level, involves exposing students to a variety of biochemical unit operations. This task is facilitated considerably by using a process simulator which features a variety of such units. Furthermore, using a process simulator as a part of teaching biochemical process design helps students explore efficiently a large number of process alternatives.

BioPro Designer is a Macintosh-based simulator designed to support the development of integrated biochemical processes in a user-friendly environment*. The current version of the software features unit operations whose applicability extends beyond biochemical applications and includes other chemical processes. Features of BioPro Designer include:

- Interactive graphical interface.
- Approximately 40 unit operations used in the biochemical and other industries.
- Material and energy balances for integrated flowsheets with recycle loops.
- Estimation of equipment size and purchase cost.

- Detailed stream and economic evaluation reports.
- Scheduling of batch and semicontinuous processes.
- On-line help.

We have used BioPro Designer in teaching senior process design and graduate biochemical process design at the New Jersey Institute of Technology (NJIT) with positive feedback from our students. The software was used to build biochemical processes, consider structural alternatives, and perform sensitivity analysis on process parameters and conditions. The students would typically report process aspects such as equipment sizing, scheduling, economic performance, and environmental impact.

Description of BioPro Designer

General Description

BioPro Designer is a sequential modular simulator. The user builds a flowheet by selecting unit operations and specifying the connectivity among them. BioPro

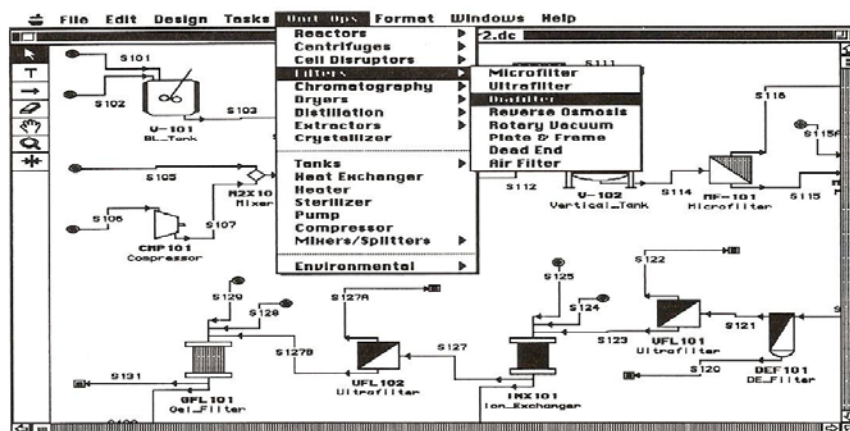


Figure 1. BioPro Designer Working Environment

* The development of BioPro Designer was initiated as a part of Dr. Petrides' Ph.D. thesis. The software is currently being extended to support the design of synthetic pharmaceutical and environmental processes.

Designer features a menu-driven, fully interactive user-interface, which is similar to other Macintosh applications. A typical BioPro Designer working environment is shown in Figure 1.

The software guides students through the steps of developing a flowsheet using the *Tasks* menu, shown in Figure 2. Before solving the mass and energy balances, BioPro Designer checks for correct flowsheet initialization, and reminds the user to complete any skipped steps.

Tasks	
Check Flowsheet	%1
Specify Mode of Operation...	%2
Initialize Components...	%3
Initialize Feed Streams...	%4
Initialize Unit_Ops...	%5
Initialize Process Scheduling...	%6
Solve M&E Balances	%M
Generate Stream Report...	
Get Cost Data...	
Perform Economic Analysis...	%E
Itemized Cost Report...	%I
Input Data Report...	
Generate Data Plot...	

Figure 2. Interactive Flowsheet Development

Unit Operations

BioPro Designer offers a wide variety of unit operations used in the biochemical, pharmaceutical, and other process industries. Table 1 shows a list of unit operations currently available.

The models of all these unit operations are algebraic. They can be specified for steady-state, batch, or

semibatch operation. Most of the design parameters and operating conditions in these unit operations have default values, which facilitates initialization and a quick preliminary assessment of operating alternatives.

A typical model is that of a *diafilter* (Figure 3). Diafilters use membrane separation to enhance purification of retained solids. A solvent is added to the retentate to help remove membrane-permeating species. Diafilters usually operate in batch mode (O'Sullivan *et al.*, 1984; McGregor, 1986).

Table 1. Unit Operations in BioPro Designer

Reaction	Phase Separation
Batch/Continuous	Centrifugal Extractor
Fermentor	Differential Extractor
Air-Lift Fermentor	Mixer-Settler Extractor
Well-Mixed Reactor	Short-Cut Distillation
Plug Flow Reactor	Flash
Fluidized Bed Reactor	Scrubber/Stripper
Cell Disruption	Crystallizer
High Pressure Homogenizer	Decanter Tank
Bead Mill	Drying/Evaporation
Mechanical Separation	Freeze Dryer
Membrane Microfilter	Tray Dryer
Membrane Ultrafilter	Fluid Bed Dryer
Diafilter	Rotary Dryer
Reverse Osmosis	Flash Evaporator
Dead-End Filter	Rotary Evaporator
Air Filter	Other Unit Operations
Plate & Frame Filter	Compressors
Rotary Vacuum Filter	Fan/Blower
Basket Filter Centrifuge	Pumps
Disc-Stack Centrifuge	Heater/Heat Exchanger
Decanter Centrifuge	Heat Sterilizer
Bowl Centrifuge	General Flow Mixer
Cyclone/Hydrocyclone	Flow/Component Splitter
Chromatography	Storage Tanks
Gel Filtration	Blending Tanks
Ion Exchange	Activated Carbon Adsorber
Reverse Phase	
Affinity	

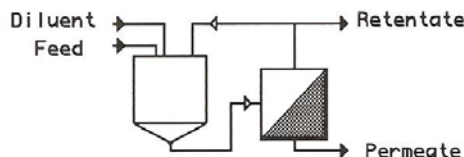


Figure 3. Icon of a Diafilter in BioPro Designer

Batch diafilter operation. Permeable solutes are cleared from the retentate by volume reduction, followed by repeated re-dilution and re-filtration in repetitive. When an equal volume reduction takes place in each stage, the final fraction of a component (F_i) remaining in the retentate is estimated by the following equation:

$$F_i = (CF)^{n(RC_i - 1)}$$

where (CF) is the concentration factor in each stage, n is the number of volume reduction stages, and RC_i is the

average rejection coefficient of solute (i). The volume of water (or other solvent) required for dilution is estimated by the following equation:

$$V_{\text{Diluent}} = V_o n \left(1 - \frac{1}{CF} \right)$$

where V_o is the initial feed volume. The value of V_{Diluent} is used to adjust the flowrate of the diluent stream.

Continuous diafilter operation. This involves adding solvent at the appropriate pH and temperature to the feed tank at the same rate as the permeate flux, thus keeping feed volume constant during processing. Permeable solutes are removed at the same rate as the flux. This mode of diafiltration is particularly useful if the concentration of the retained solute is too high to permit effective discontinuous diafiltration operations for purification. The fraction of solute remaining in the retentate is estimated by the following equation:

$$F_i = e^{-(VPR)(1-RC_i)}$$

where (VPR) is the volumetric permeation ratio, defined as follows:

$$VPR = \frac{\text{Volume of Liquid Permeated}}{\text{Initial Feed Volume}}$$

The volume of water (or other solvent) required for dilution is estimated by the following equation:

$$V_{\text{Diluent}} = (VPR)V_o$$

where V_o is the initial feed volume. The value of V_{Diluent} is used to adjust the flowrate of the diluent stream as in the case of discontinuous diafiltration.

Unit operations are initialized interactively through a series of dialog windows. Figure 4 depicts the initialization windows for a diafilter. The radio buttons indicate alternative modes of operation. The numbers already present in the windows are the default values suggested by BioPro Designer.

Production of Sodium Nitriloacetate (NTAN) – A Senior Design Project at NJIT.

This example is drawn from the specialty chemical industry. Students were asked to synthesize a process for the production of sodium nitriloacetate (NTAN). They were also asked to assess the economic viability and the environmental impact of their design.

NTAN is used as a detergent builder, i.e. an additive to the detergent whose role is to reduce water hardness. NTAN is produced in three stages: hexamethylene (HMTA) synthesis, nitrile synthesis (NTA), and nitrile saponification (NTAN).

The NTAN production flowsheet shown in Figure 5 has been adapted from the solution of one student group using BioPro Designer. The design basis of the project is 50 million lbs/year.

HMTA is produced from aqueous solutions of ammonia and formaldehyde in reactor R-101. NTA is produced from HMTA, hydrogen cyanide, and formaldehyde in the presence of sulfuric acid. The reaction is carried out in a well-mixed reactor and a plug flow reactor in series (R-102 and R-103 respectively). The effluent from the reactor passes through a rotary vacuum filter (RF-101) where NTA is retained in the solid phase. NTAN is produced from saponification of NTA with sodium hydroxide. The reaction takes place in reactors R-104 and R-105. The effluent from these

DF-101 Design Data	
Molecular Weight Cut Off (Daltons):	30000.0
Average Filtrate Flux (L/m ² -h):	20.0
Concentration Factor:	2.00
Max. Solutes Conc. in Retentate (v/v):	0.60
Outlet Streams Temperature (°C):	25.00
Mode of Operation ☒ Discontinuous Number of Stages: 2.0 ☐ Continuous Volumes Permeated: 2.0	
Power Consumption (kW/m ²):	0.20
Membrane Replacement (operation h):	2000.0
Membrane Unit Cost (\$/m ²):	200.0
Membrane Area (m ²):	0.00
Next Cancel Show Cost	

Figure 4 (a). First Diafilter Initialization Window

DF-101 Design Data

Component Rejection Coefficient (RC):

Component	RC
Ecoli	1.00
Product	0.000
Biomass	1.000
H2O	0.000
CO2	0.000
Glucose	0.000
NH3	0.000
O2	0.000

Product

Active Product:

Denatured Product:

Denaturation Fraction:

Product

Previous

OK

Cancel

Figure 4 (b). Second Diafilter Initialization Window

reactors, contains ammonia as a by-product, which is removed by distillation (C-101). NTAN is recovered by a series of crystallization and filtration steps (M-101, RF-102, M-102, and RF-103). The process is completed with a drying step in M-103.

BioPro Designer provides the results of the material balance calculations in a stream report, which includes

temperature, pressure, and flowrates for each component in the stream. The stream report also includes an overall material balance. Parts of this report are shown in Table 2.

The economic reports are designed to assist in screening out certain process alternatives. Their accuracy is within $\pm 25\%$. Sizing and costing information is reported in a variety of formats. The first table of the

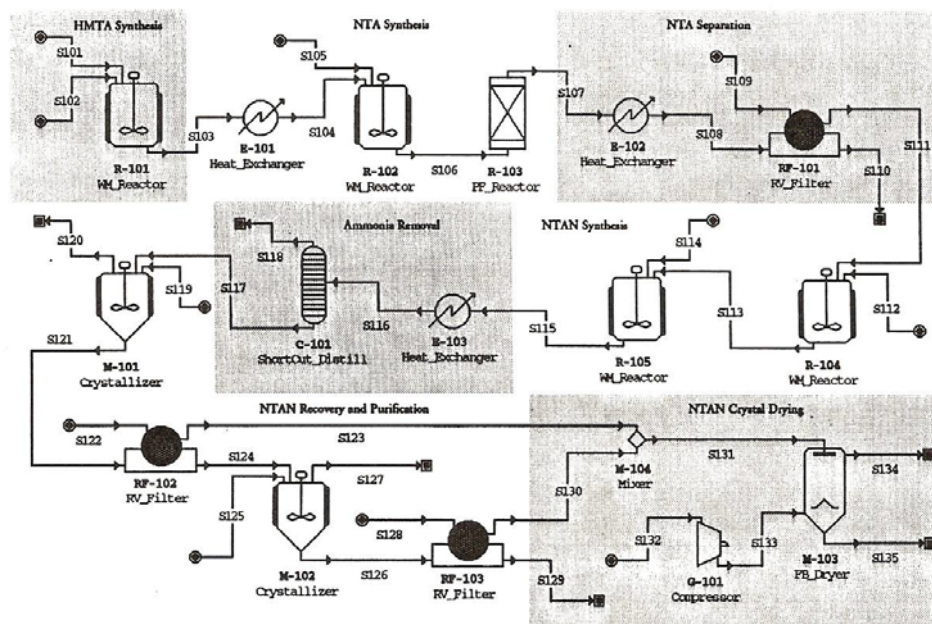


Figure 5. Production of NTAN Designed by Senior NJIT Students

main report includes the size, material of construction, and cost for each unit in the process (Table 3). The rest of the main report provides information on direct fixed capital, cost of labor, raw materials, utilities, and waste treatment. This information is used to perform an overall profitability analysis and report the expected return on investment and the project payback time.

BioPro Designer also reports the cost per product mass for each individual unit. This information is useful for teaching retrofit design of a chemical processing

facility. As a part of their term project, students were instructed to focus their redesign efforts on the process subsystems which contribute the larger cost or waste to the process. In this case they considered recycling the ammonia produced during the NTAN synthesis step back to the HMTA synthesis step, where ammonia is a reactant.

BioPro Designer presents the process schedule in the form of a Gantt chart. Students can modify the scheduling information directly onto the graphics of the chart.

Table 2 (a). Parts of BioPro Designer's Stream Report

STREAM NAME	S101	S102	S103	S104	
SOURCE	FEED	FEED	R-101	E-101	...
DESTINATION	R-101	R-101	E-101	R-102	

STREAM PROPERTIES					
ACTIVITY	U/ml	0.0	0.0	0.0	0.0
TEMP	°C	25.0	25.0	38.0	10.0
PRES	BAR	2.0	2.0	2.0	2.0

WEIGHT PERCENT					
NH3	30.0000	0.0000	0.4740	0.4740	
HCHO	0.0000	37.0000	1.2617	1.2617	
H2O	70.0000	63.0000	79.6157	79.6157	
HMTA	0.0000	0.0000	18.6486	18.6486	
HCN	0.0000	0.0000	0.0000	0.0000	
NTA	0.0000	0.0000	0.0000	0.0000	
NAOH	0.0000	0.0000	0.0000	0.0000	
NTAN	0.0000	0.0000	0.0000	0.0000	
H2SO4	0.0000	0.0000	0.0000	0.0000	
AIR	0.0000	0.0000	0.0000	0.0000	
NTAN-xtal	0.0000	0.0000	0.0000	0.0000	

COMPONENT FLOWRATES (kg/h)					
NH3	199.9943	0.0000	9.9364	9.9364	
HCHO	0.0000	528.9926	26.4496	26.4496	
H2O	466.6543	900.7170	1669.0310	1669.0310	
HMTA	0.0000	0.0000	390.9412	390.9412	
HCN	0.0000	0.0000	0.0000	0.0000	
NTA	0.0000	0.0000	0.0000	0.0000	
NAOH	0.0000	0.0000	0.0000	0.0000	
NTAN	0.0000	0.0000	0.0000	0.0000	
H2SO4	0.0000	0.0000	0.0000	0.0000	
AIR	0.0000	0.0000	0.0000	0.0000	
NTAN-xtal	0.0000	0.0000	0.0000	0.0000	
=====					
TOTAL	666.6486	1429.7096	2096.3582	2096.3582	
=====					

Table 2b. BioPro Designer's Stream Report Continued

OVERALL MATERIAL BALANCE (kg/Year) (Hours per Year = 8000)			
COMPONENT	IN	OUT	Δ (OUT-IN)
NH3	1599954.48	4631999.71	3032045.23
HCHO	8675478.40	638601.74	-8036876.66
H2O	47861718.88	47868828.60	7109.72
HMTA	0.00	2964.84	2964.84
HCN	7254282.56	26664.30	-7227618.26
NTA	0.00	11957.72	11957.72
NAOH	11240239.36	547324.50	-10692914.86
NTAN	0.00	229060.16	229060.16
H2SO4	2188442.24	2188442.24	0.00
AIR	107716560.00	107716560.00	0.00
NTAN-xtal	0.00	22676945.40	22676945.40
TOTAL	186536675.92	186539349.21	2673.29

Table 3. Sizing and Costing of Major Equipment (Part of the Economic Report)

Quantity/ Stand-by	Description	Unit Cost (\$)	Cost (\$)
1/0 R-101	Agitated Reactor Vol = 4.93 m ³ , SS316, 2.10 kW	64000	64000
1/0 E-101	Heat Exchanger A = 4.30 m ² , SS316, -51807.8 kcal/h	4000	4000
1/0 R-102	Agitated Reactor Vol = 5.48 m ³ , SS316, 2.33 kW	67000	67000
1/0 R-102	Plug Flow Reactor Vol = 8.46 m ³ , SS316	36000	36000
1/0 E-102	Heat Exchanger A = 11.49 m ² , SS316, -267467.7 kcal/h	8000	8000
1/0 RF-103	Rotary Vacuum Filter A = 10.5 m ² , SS316, 0.00 kcal/h	65000	65000
1/0 G-101	Centrifugal Compressor ΔP = 1.0 bar, CS, 1247.01 kW	871000	871000
1/0 G-101	Fluid Bed Dryer CS, Duty = 1961142 kcal/h	425000	425000
	Cost of Unlisted Equipment 20.0 % of Total		476000
TOTAL EQUIPMENT PURCHASE COST			2380000

Discussion and Conclusion

Senior undergraduate and graduate students have used BioPro Designer to analyze and evaluate several integrated processes. The products ranged from specialty to commodity chemicals, and production processes included biological as well as synthetic pathways.

One project was the production of citric acid, a major commodity chemical produced via a biological pathway. Students used the software to develop and examine several flowsheets, based on alternative feed preparation, reaction, separation and recycling schemes. They were exposed to a wide variety of biochemical unit operations, considered "what if" questions, and examined the economic and environmental impact of process modifications.

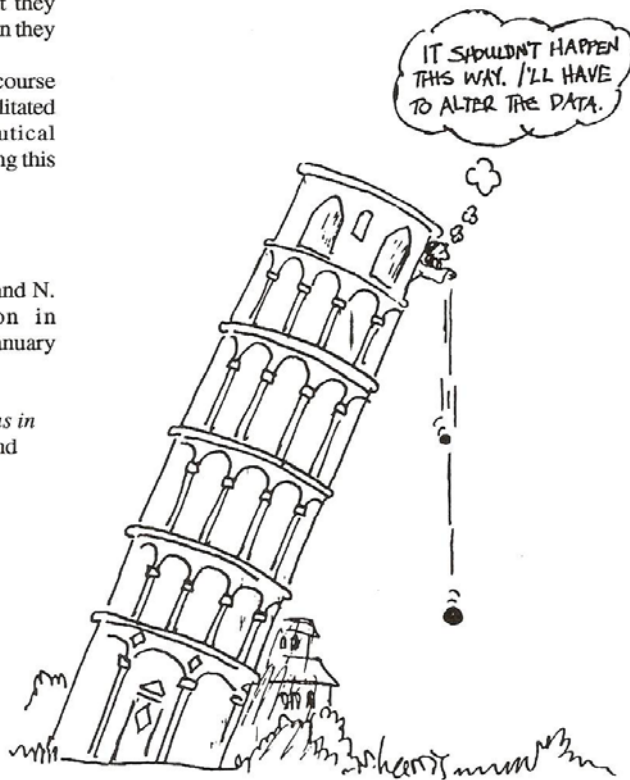
The feedback of the senior design students on using BioPro Designer was positive. They mentioned that it was easy to learn the software and they felt that they were able to consider more process alternatives than they would if BioPro Designer were not available.

BioPro Designer was also used in a graduate course on pharmaceutical technology. In that course, it facilitated presenting the process aspect of pharmaceutical processes, which is often overlooked, when teaching this field.

References

O'Sullivan, T. J., A. C. Epstein, S. R. Korchin, and N. C. Beaton. Applications of Ultrafiltration in Biotechnology, *Chemical Engineering Progress*, January 1984.

McGregor, W. C. (editor). *Membrane Separations in Biotechnology*, Marcel Dekker, Inc., New York and Basel, 1986.



The Physics Teacher Vol. 30, March 1992

POLYMATH Numerical Computation Package

New Release - Version 3.0

*By Michael B. Cutlip, University of Connecticut
Mordechai Shacham, Ben Gurion University of the Negev, Israel*

The POLYMATH package has been significantly upgraded, and the latest version is available from CACHE. Some of the most important new features include the following:

- Speed of Execution 15X to 50X previous version
- Supports floating point processors when available
- Automatically adjusts to user's display
- Much improved and faster printing (no more screen display copies only)
- Supports all major printers including Epson, HP, IBM, OkiData, Toshiba, PostScript, LaserJets, Dot Matrix, BubbleJet, Plotters, etc.
- Same user interface with much more convenient standard editing
- New file import and export capabilities with spreadsheet compatibility
- Upper and lower cases now allowed for user variables
- Much improved user library problem storage with conversion utility from previous version
- Network support
- Printing option to standard graphics files - TIFF, Gem IMG, WPG, Windows 3 BMP, etc.
- Fully functional as a DOS application under Windows
- Fully functional on Power Macintosh computers using SoftWindows
- A single personal copy is provided on the CACHE CD-ROM
- Hardcopy Manual plus Manual on disk in PDF file for use with Acrobat Reader by Adobe
- Companion Book Available - "Numerical Solution of Chemical Engineering Problems Using POLYMATH"

Significant New Capabilities - POLYMATH Polynomial, Multiple Linear and Nonlinear Regression Program

Major changes have been made in the area of data regression. A new spreadsheet-like data entry table allows users to conveniently transform data in almost any way

and also perform calculations on columns of data prior to regression. This very helpful in situations where data columns must be treated before linear or polynomial regression. Complete statistical output is now available for all regressions including polynomials. Linear regressions and polynomial regressions have options where they can be forced through the origin in cases where this is desirable.

Important New Feature - General Nonlinear Regression

Perhaps the most important new feature is a general NONLINEAR REGRESSION CAPABILITY which uses the robust Levenberg-Marquardt algorithm. This new option allows the user to input any form of an expression for the data containing up to five parameters. The user interface on this new capability is very easy to use, and the algorithm converges quite well from even poor initial estimates for the parameter values. Statistical output is also provided for this option. This POLYMATH capability can greatly assist undergraduate students in modeling and statistics.

Legitimate Student Copies of POLYMATH

The inexpensive POLYMATH site license (discussed below) allows every student to have a copy of POLYMATH for their use on any personal computer. Universities can give copies to interested faculty and provide POLYMATH in personal computer labs under this license for no additional cost. Users will receive updated versions of POLYMATH for no additional costs.

Why Use POLYMATH?

POLYMATH really is very easy to use. Students and faculty agree on this! There is usually no need to refer to the manual. The software is menu driven so that all the current options and the necessary keypresses are indicated on the screen. Nothing must be memorized! Students and other users really like the simplicity of POLYMATH. It is very intuitive, and the equation entry almost identical to the mathematical expression used in problem solving. There is no other software which must be purchased with POLYMATH. It will run on almost

any IBM-compatible personal computer including the older machines. Unlike other mathematical packages, POLYMATH gives details on the algorithms and techniques that are used in problem solution.

POLYMATH Overview

POLYMATH is very useful as general problem solving software throughout the Chemical Engineering curriculum. POLYMATH improves faculty and student ability to solve more realistic numerical problems which reduces emphasis on the details of the computing. It can also be used to support courses in numerical analysis as details on the numerical methods are given in help sections of the programs.

POLYMATH Programs:

- **Algebraic Equation Solver** - This program can solve up to a combination of twelve simultaneous nonlinear equations and explicit algebraic expressions. All equations are checked for correct syntax and other errors upon entry. Equations can easily be modified, added, or deleted. Multiple roots are given for a single equation. A separate simple linear equation solver handles up to 6 simultaneous equations.
- **Differential Equation Solver** - This program enables the numerical integration of up to twelve nonlinear ordinary differential equations and explicit algebraic expressions. The format is almost identical to the written differential equations. All equations are checked for syntax upon entry. Equations are easily modified. Initial values must be provided. Undefined variables are identified. The integration method and stepsize are automatically selected. Graphical output of problem variables is easily obtained using automatic scaling.
- **Curve Fitting and Regression Program** - This program allows users to input (or read from a file) up to 30 columns of data with up to 100 data points per column. The data can be manipulated by defining expressions the names of previously defined columns. This allows great freedom in data manipulation prior to regression (polynomial, multiple linear, and nonlinear) or cubic spline fitting and interpolation. Fitted curves (polynomial and splines) can be interpolated, differentiated and integrated. Graphical output of the fitted curves and expressions is provided, and a statistical analysis of the coefficients is given.

POLYMATH Input/Output

All programs provide the ability to read and write to DOS files with the option of the creation of convenient

user libraries. Fast printing of problems, data, and output is available to all major printers and plotters plus various standard output files can be created for incorporation into documents.

POLYMATH Execution

POLYMATH now executes very quickly utilizes floating processors when they are available. The programs automatically adjust to the graphics monitors which are used. No additional software or compilers are used. The software is a DOS application which can also be executed as a DOS application in Windows. Automatic installation to individual IBM compatible personal computers and to networks is supported. Memory requirement is 550 Kb, and hard disk installation requires 1 Mb.

POLYMATH is Useful in the Following Courses:

- Material and Energy Balances
- Thermodynamics
- Data Correlation
- Fluid Mechanics
- Separation Processes
- Chemical Reaction Engineering
- Heat and Mass Transfer
- Process Dynamics and Control

Recent Papers Related to POLYMATH

The following current publications demonstrate some potential applications and some of the capabilities of POLYMATH:

Shacham, M., N. Brauner and M. Cutlip, "Applications of Small Scale Interactive Numerical Simulation Packages in Chemical Process Design", CHISA'93 Conference, Prague, Czech Republic, September (1993).

Shacham, M., N. Brauner, and M. B. Cutlip, "Exothermic CSTRs - Just How Stable are the Multiple Steady States?", Chemical Engineering Education, 28, 1, pp. 30-35 (1994).

Brauner, N., M. Shacham, and M. B. Cutlip, "Application of an Interactive ODE Simulation Program in Process Control Education", Chemical Engineering Education, 28, 2, pp. 130-135 (1994).

Shacham, M., N. Brauner and M. B. Cutlip, "Applications of Small Scale Simulation Packages in Process Operations", Proceedings of the Second International Conference on Foundations of Computer Aided Process Operations of July 1993, pp. 469-474, CACHE Corporation, Austin, TX (1994).

Shacham, M., N. Brauner and M. B. Cutlip, "Critical Analysis of Experimental Data, Regression Models and Regression Coefficients in Data Correlation", Proceedings of the Fourth International Conference on Foundations of Computer Aided Process Design of July 1994, CACHE Corporation, Austin, TX, in press.

Shacham, M., M. B. Cutlip and N. Brauner, "General Purpose Software for Equation Solving and Modeling

of Data", 25th Anniversary Monograph, CACHE Corporation, Austin, TX, in press.

POLYMATH Trial Offer

You may request this package from CACHE for testing and evaluation. If you decide to obtain POLYMATH for a three month trial period, please be aware of the conditions set forth in the order form below.

POLYMATH ORDER FORM

1. You may reproduce the program as many times as you like for students and other faculty.
2. Your department chairman will be informed of the testing.
3. If you decide to use POLYMATH in your department after three months, supporting departments will be billed for \$125.00 and \$75.00 for each successive year thereafter. This fee covers any updates or new versions. CACHE nonmember institution rates are an initial \$150 with an annual fee of \$100.
4. If you decide not to use POLYMATH after 3 months, you must return (or certify you have erased) all copies made.

Industrial site licenses are \$300 with an annual fee of \$200. This includes distribution, computer laboratory use, and unlimited personal computer copies to employees.

Individual student copies of POLYMATH are \$25.

Please send me a copy of POLYMATH for the IBM/PC. I have read and understood the conditions described above.

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Picles 4.0 and the Case of the Jacketed CSTR

By Douglas Cooper¹ and Jerry Bieszczad, University of Connecticut

Introduction

Picles™, the Process Identification and Control Laboratory Experiment Simulator, is IBMPC compatible software now being used in more than 50 process dynamics and control courses around the world. Picles is an easy-to-use training simulator that provides hands-on experience to those studying this often abstract and mathematical subject. With over a half-dozen companies now using the software for employee training, Picles truly offers "real-world" experiences to students.

Picles contains a series of case studies, animated in color-graphic display, for self-paced or faculty guided learning. Users can manipulate process variables in open loop to obtain pulse, step, sinusoidal or ramped test data. Picles can record this data as printer plots or disk files for process identification and controller design. Digest™, companion software to Picles, is one package well suited for this identification and design task. After designing a controller, return to Picles and immediately evaluate and improve upon the design for both set point tracking and disturbance rejection.

A pre-release version of Picles 4.0 is being alpha tested this fall in the classrooms of a dozen adventurous faculty. The new version retains all capabilities of the previous release and adds a host of new ones. Major additions include a multiple steady state jacketed CSTR process which can be operated either in a single loop control mode or a cascade control mode; a digital controller for studying dead-beat, Dahlin and other z-domain algorithms; an improved data plotting facility to make homework solutions more convenient to document; and an expanded on-line help facility.

After a brief review of Picles' features, this article explores one case study possible with the new jacketed CSTR process. The discussion compares the challenges of the single loop controller design with those of the cascade control architecture. A third comparison using a feed forward architecture is left for a student homework assignment. As part of the discussion, the use of the Digest dynamic modeling and controller design package is also demonstrated.

The Picles Case Studies

Previous CACHE Newsletters describe the Picles processes in some detail. The new Picles 4.0 adds a multiple steady state jacketed CSTR process with a single loop or cascade control configuration to yield the case study options:

One-Input One-Output Case Studies:

Gravity Drained Tanks, Heat Exchanger, Pumped Tank, Mystery Processes

Ideal Transfer Function Case Study:

Design a Process

Multiple Steady State Case Study:

Jacketed CSTR

Two-Input One-Output Cascade Case Study:

Jacketed CSTR

Two-Input Two-Output Multivariable Case Study:

Distillation Column

The Picles Controllers

The Picles control algorithms can be custom tuned and implemented in only a few key strokes. Available controllers, which permits a broad variety of concepts to be explored, include:

Manual Control
P-Only Control
I-Only Control
Velocity PID Control with Derivative on Measurement
Velocity PID Control with Derivative on Error
Position PID Control (no windup protection)
Velocity PID with Smith Predictor
Velocity PID with Feed Forward
Velocity PID with Decouplers
Digital Sampled Data Controller

The Distillation Column and the Jacketed CSTR Cascade case studies have two control loops. Users can mix the P-Only through full PID algorithms for the controllers in these applications. Decouplers are also available for the Distillation Column.

¹ Author to whom all correspondence should be addressed

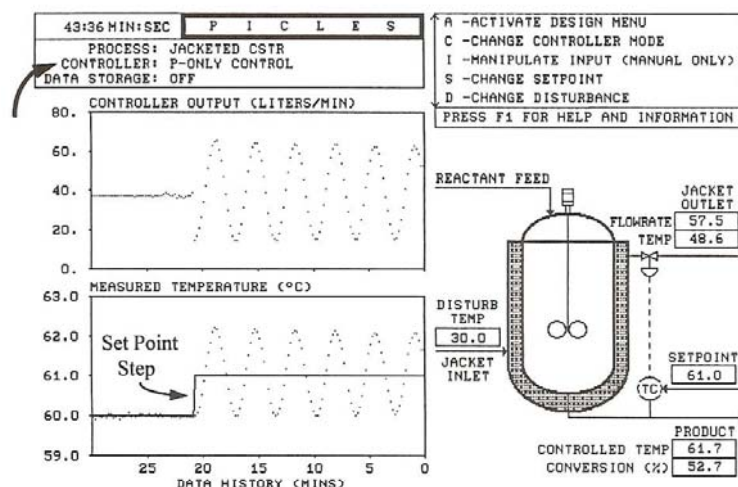


Figure 1 - Single Loop Jacketed CSTR Process at Limit of Stability Under P-Only Control

The Jacketed CSTR Process

The Jacketed CSTR Process, shown in Figure 1 for the single loop case, is a stirred reactor in which the first order irreversible exothermic reaction $A \rightarrow B$ occurs. Residence time is constant in this perfectly mixed reactor, so the steady state conversion of reactant A from the reactor can be directly inferred from the temperature of the reactor product stream. To control reactor temperature, the vessel is enclosed with a jacket through which a coolant passes.

As shown in Figure 1, the manipulated process input variable is coolant flow rate through the jacket. The measured/controlled process output variable is product stream temperature. The disturbance variable in this simulation is the inlet temperature of coolant flowing through the jacket.

This CSTR has multiple steady states. Picles initializes the process at a middle, unstable, steady state temperature. Any open loop manipulation of the coolant flow rate or disturbance coolant inlet temperature initiates an excursion to either the upper or lower stable operating temperature.

The process is modeled following developments similar to those presented in Luyben (1990) and Smith and Corripio (1985). Assuming an irreversible first order reaction ($A \rightarrow B$); perfect mixing in the reactor and jacket; constant volumes and physical properties; and negligible heat loss, the model is expressed:

Balance on Mass of Reactant A:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - kC_A$$

Energy Balance on Reactor Contents:

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) - \frac{\Delta H_R}{\rho C_P} kC_A - \frac{UA}{V\rho C_P}(T - T_J)$$

Energy Balance on Jacket:

$$\frac{dT_J}{dt} = \frac{UA}{V_J\rho_J C_{PJ}}(T - T_J) + \frac{F_J}{V_J}(T_{J0} - T_J)$$

Reaction Rate Coefficient:

$$k = k_0 e^{-E/RT}$$

Picles also has first order lags on the manipulated and disturbance variables to simulate valve dynamics. Normally distributed random error, which can be adjusted by the user and has a default value of ± 3 standard deviations equal to 0.1 °C, is added to the measured process output (product stream temperature) to simulate modest measurement noise.

Objective of This Case Study

The objective of case study presented here is the design of a controller which will maintain the CSTR product stream at the unstable steady state temperature while successfully rejecting disturbances introduced through changes in the cooling jacket inlet temperature. Note that a host of other studies could also be explored using the options available in Picles.

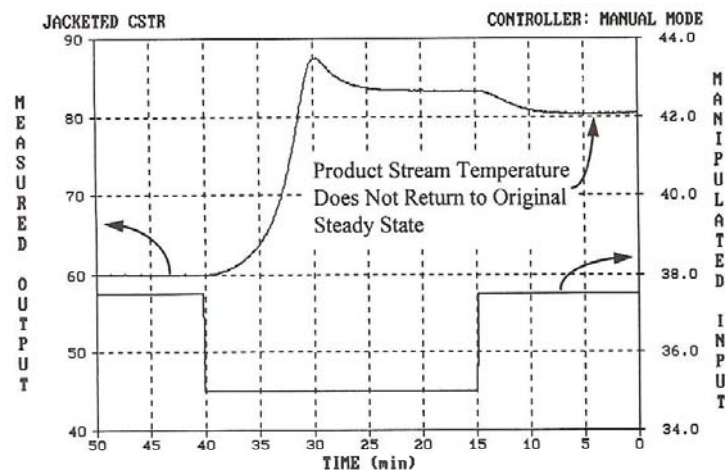


Figure 2 - CSTR Excursion to Upper Stable Steady State

Single-Input Single-Output Solution

Open Loop Modeling

The classical approach to designing a controller begins with a process identification study. This procedure is carried out in Picles the same way one would proceed on a real plant:

- 1) the manipulated process input variable is either stepped or pulsed in manual mode (open loop),
- 2) the measured process output response is recorded,
- 3) a low order linear dynamic model is fit to the process input/output relationship, and
- 4) the resulting model parameters are used in tuning correlations to determine initial controller settings.

One challenge of the Jacketed CSTR is that, for the objective stated above, this classic procedure fails.

Figure 2 shows a step test plot generated using the Picles plotting facility. This plot shows that the manipulated process input variable, jacket coolant flow rate, is initialized at 37.5 liters/minute. During the identification study, the jacket coolant flow rate is stepped down to 35 liters/minute for about 20 minutes and then returned to its original value.

The measured output of the process, product stream temperature, begins at 60 °C. This temperature corresponds to the CSTR unstable steady state for the Picles startup conditions. After the first input manipulation, the temperature spikes to over 85 °C. When the manipulated input returns to its original value,

however, the measured variable does not return to the original steady state. Rather, process operation has moved to the upper stable operating region due to the step test.

The process input/output data generated from this open loop test contains influences from two different steady state operating regimes. Consequently, a dynamic model regressed from this data will poorly describe the process behavior at either operating regime, making this model of little value for controller design.

Closed Loop Modeling Via Ziegler-Nichols

Open loop pulse tests are desirable methods of process identification in real plants because the process usually returns to its original operating point relatively quickly. Thus, input/output dynamic data, sought for controller design, is obtained with minimal off-specification production. Since this approach fails for the Jacketed CSTR Process, the next choice is a closed loop identification study.

The classical approach to closed loop process identification is that proposed by Ziegler and Nichols (e.g. Stephanopoulos, 1984; Seborg *et al.*, 1989). In this method, the procedure is to:

- 1) Implement a P-Only controller,
- 2) Perturb the process near the desired point of operation,
- 3) Search by trial and error for the smallest value of the controller gain which effects sustained oscillations in the measured output. These oscillations should neither grow nor die and the manipulated input should remain unconstrained.

- 4) The controller gain at this condition is the ultimate gain. The period of oscillation in the measured variable at the ultimate gain is called the ultimate period.
- 5) The ultimate gain and period are then used in Ziegler-Nichols correlations to determine initial PID settings.

The disadvantage of Ziegler-Nichols is that the process must literally be brought to the brink of instability. For real processes, such a notion is very unpopular with operating personnel.

Notwithstanding this disadvantage, Figure 1 shows the CSTR at the limit of stability near the unstable steady state operating regime. The bold arrow on the figure indicates that a P-Only controller is in place. The Picles design menu (not shown) reveals that the ultimate gain for the process is -23 liters/(minute °C). Using the Picles plotting facility, it is determined that the ultimate period in the measured output is about 210 seconds. The Ziegler-Nichols correlations thus yield the PID tuning parameters:

Controller Gain, $K_C = -13.8$ liters/(minute °C)

Reset Time, $\tau_I = 105$ seconds

Derivative Time, $\tau_D = 26.3$ seconds

Unfortunately, implementation of a PID (velocity mode with derivative on measurement) controller with these parameters results in erratic closed loop process behavior. The derivative time computed from the Ziegler-

Nichols correlations puts a very large weight on the discrete derivative computation of the algorithm. This amplifies the very modest measurement noise and produces irregular, wandering regulation rather than a desirable tight control. It is interesting to note that if the Picles design menu is used to remove all measurement noise, the Ziegler-Nichols tuning is stable and produces reasonable regulatory performance.

Final Resort - Trial and Error

Although too much derivative action causes problems for this process, the same is true for too little derivative action. If a PI algorithm is used with the appropriate Ziegler-Nichols tuning, the tendency of the process to seek the stable upper or lower steady states overwhelms the control capability of the algorithm, producing significant and slowly damping oscillations whenever the process is perturbed.

Hence, with Ziegler-Nichols tuning as a starting point for PID control, on-line trial and error tuning appears necessary to produce reasonable regulatory performance. Because excessive derivative action is the culprit for the erratic performance, the first step is to back down on this parameter. With less derivative action, the integral time must be increased to reduce its tendency to produce oscillation (integral time is in the denominator, so a larger value decreases its weighting in the algorithm computations).

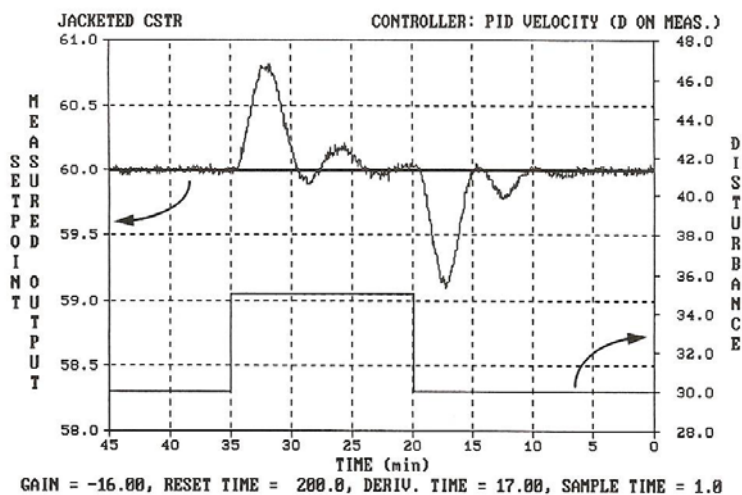


Figure 3 - Regulatory Performance of the Single Loop Jacketed CSTR Under PID Control

After some tinkering, reasonable regulatory performance is obtained using the PID parameters:

Controller Gain, $K_C = -16.0$ liters/(minute $^{\circ}\text{C}$)

Reset Time, $\tau_I = 200$ seconds

Derivative Time, $\tau_D = 17.0$ seconds

Figure 3 shows the single loop controller performance using these tuning parameters. This figure shows that the measured product temperature is initialized at the unstable steady state value of 60°C . Two step disturbances occur where the jacket coolant temperature is stepped from its initial value of 30°C up to 35°C and then 15 minutes later back down to 30°C . The single PID controller maintains the product stream temperature near the constant set point of 60°C (solid line) and ranges during the transients from about 59.2°C to about 60.8°C .

Cascade Control Solution

The open loop behavior of the Cascade Jacketed CSTR is identical to the single loop case. The only difference between the two is the controller architecture. The Picles graphic of the cascade control architecture is shown in Figure 4. Figure 5 shows a block diagram of this same architecture. As shown in these figures, a control cascade consists of two measurements, two controllers, but only one final control element - the same final control element as in the single loop case study.

In the Picles CSTR, the secondary or inner process of the cascade is the cooling jacket. The manipulated process input variable of the secondary loop is the cooling

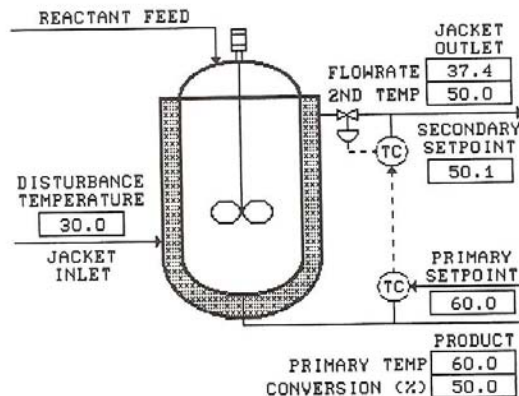


Figure 4 - Picles Graphic of Cascade Control Architecture

jacket flow rate and the measured process output variable is coolant temperature out of the jacket. The primary or outer process is still the CSTR and the measured process output variable is still the product stream temperature. As shown in Figure 5, however, notice that the manipulated process input variable for the primary loop is the set point to the secondary loop.

The advantage of a cascade approach is that a secondary controller can begin compensating for disturbances even before the primary measured variable

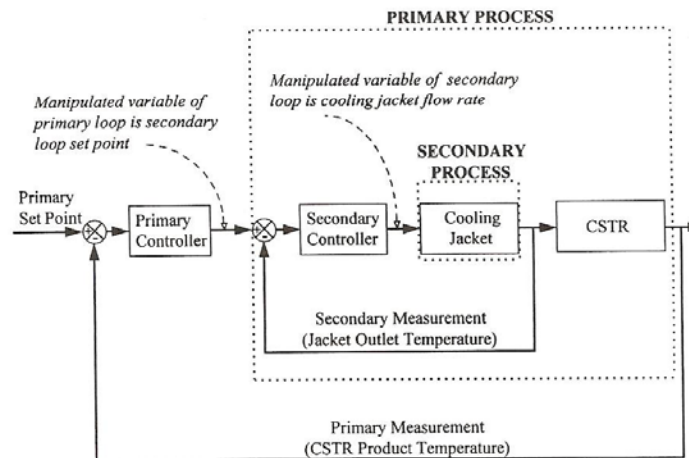


Figure 5 - Block Diagram of Jacketed CSTR Cascade Architecture

is affected. A requirement for effective cascade control is that the secondary loop has much faster dynamics (a smaller time constant) than that of the primary loop. This is true for the Jacketed CSTR as the jacket coolant temperature control loop has much faster dynamics than the product stream temperature control loop.

For controller tuning, the classical approach is to first implement the secondary controller using a simple algorithm, such as a P-Only controller, while the primary loop is in manual mode. After validating the controller performance of the secondary controller, it is left in automatic and the primary controller is then designed.

Secondary Loop Control

Just as in the previous single-input single-output discussion, an open loop identification study cannot be used because of the tendency of the process to seek one of the stable steady states. When the closed loop Ziegler-Nichols method is employed for the secondary control loop, it is found that the P-Only gain can be set to its extreme value (-999) in the Picles design menu without causing significant oscillation in the measured jacket outlet temperature. Such behavior is characteristic of a true first order process.

Even though an extreme controller gain maintains stability, there is a practical disadvantage to using such a tuning and that is that manipulations of the final control element are excessive and valve wear becomes a concern. Using engineering judgment, an intermediate P-Only controller gain, $K_C = -100$ liters/(minute °C), is chosen here to balance controller performance with valve "chatter." The secondary loop design is now complete. The controller is left in automatic and the primary controller design is considered.

Note that using a P-Only controller on the secondary loop results in offset for measured jacket outlet temperature. This does not present a problem, however, if a controller with integral action is chosen for the primary loop. After all, a well regulated CSTR product stream temperature is the ultimate objective of this case study.

Primary Loop Control

One result of having the secondary loop under P-Only control is that the primary loop becomes stable in manual mode. Hence, an open loop pulse or step test identification study can be performed. Following the procedure described earlier, the manipulated process input variable of the primary loop, which in this case is the secondary loop set point, is stepped from its initial steady state value of 50 °C up to 55 °C. The Picles data file storage utility is used to collect data from the measured product stream temperature as it responds to this manipulation.

Using DIGEST for Dynamic Modeling

The next step in the controller design procedure is to fit a low order linear dynamic model to this process input/output data. There are a host of approaches to this model fitting problem, ranging from graphical procedures to sophisticated regression packages.

One software package well suited for this model fitting task is Digest, a companion product to Picles. Digest can import ASCII files containing dynamic data from Picles, other software packages and even from a real plant. The data must be in ASCII tabular form with data columns separated by tabs, commas or spaces. Simple Digest commands are used to mark which data column contains the manipulated process input data, which column contains the measured process output data, and which column contains the time data. The linear models available in Digest include First Order, First Order Plus Dead Time, Second Order and Second Order Plus Dead Time dynamic forms.

Digest then fits the process gain, time constant(s) and dead time (if applicable) to the data by minimizing the sum of the squared error (SSE) between the actual process output and the predicted model output response when using the manipulated input data contained in the file. In computing the SSE, Digest operates according to the following assumptions:

- 1) The process is at steady state before the dynamic event occurs,
- 2) The first data point in the file is a good median value of the initial steady state, and
- 3) The time increment between the data points is constant.

Figure 6 shows the Digest fit of a first order plus dead time (FOPDT) model to the dynamic data collected during the primary loop step test described above. Digest fits the model to the product stream temperature in spite of the oscillations in the measured variable. Digest performs equally well for pulse tests and even closed loop identification studies. In this case, The model parameters computed by Digest are:

Process Gain, $K_p = 1.944$ (°C of product stream)/
(°C coolant temperature)
Overall Time Constant, $\tau_p = 25.79$ seconds
Apparent Dead Time, $\theta = 85.19$ seconds

Controller Tuning From Model Parameters

The next step is to use these dynamic model parameters in correlations to obtain initial estimates for controller tuning. Digest contains a number of such correlations, including IMC (internal model control),

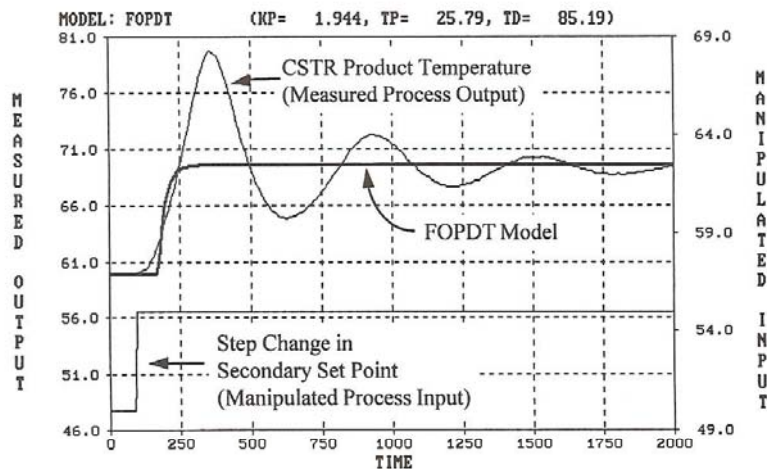


Figure 6 - Digest Fit of a FOPDT Model to Dynamic Data from a Primary Loop Step Test

Cohen-Coon, IAE (integral of absolute error), and ITAE (integral of time weighted absolute error) and will compute the tuning parameters for a P-Only, PI or PID algorithm at user request. Figure 7 shows such a computation for the above FOPDT model parameters for a PID controller.

Arrows in Figure 7 point to PID tuning parameters computed from ITAE and IAE relations for the case of disturbance changes (Smith and Corripio, 1985). Since disturbance rejection is the objective in this study and lacking any motivation to choose one of the relations

over the other, average values are employed as initial tuning parameters:

Controller Gain, $K_C = 0.24$ ($^{\circ}\text{C}$ of coolant stream)/($^{\circ}\text{C}$ of product stream)

Reset Time, $\tau_I = 72.9$ seconds

Derivative Time, $\tau_D = 40.3$ seconds

Figure 8 shows the closed loop system performance using these tuning parameters. Just as in Figure 3, this figure shows that the primary measured variable, the product stream temperature, is initialized at the unstable steady state value of 60°C . Two step disturbances occur where the jacket coolant temperature is stepped from its initial value of 30°C up to 35°C and then 15 minutes later back down to 30°C .

The cascade architecture performs markedly better than the single loop case in maintaining the product stream temperature near the constant set point of 60°C (solid line). In this cascade case, the transients in the measured variables only range from about 59.7°C to about 60.2°C .

Homework - Feed Forward

Does this close the Case of the Jacketed CSTR? Not by a long shot! There is at least one more Picles study required to complete this particular sequence. That entails returning to the single loop Jacketed CSTR simulation and demonstrating the disturbance rejection capabilities of the Velocity PID with Feed Forward algorithm. Like the cascade architecture, feed forward requires two measurements (feed forward directly measures the

TUNING PARAMETERS	
Controller Mode: PID	
Cohen-Coon	
Controller Gain =	8.336
Reset Time =	112.8
Derivative Time =	19.35
ITAE (for Set Point Changes)	
Controller Gain =	8.179
Reset Time =	83.87
Derivative Time =	24.18
ITAE (for Disturbance Changes)	
Controller Gain =	8.225
Reset Time =	73.98
Derivative Time =	32.26
IAE (for Set Point Changes)	
Controller Gain =	8.198
Reset Time =	83.83
Derivative Time =	26.75
IAE (for Disturbance Changes)	
Controller Gain =	8.246
Reset Time =	71.89
Derivative Time =	48.36

Figure 7 - Digest Tuning Parameters for FOPDT Parameters of Figure 6

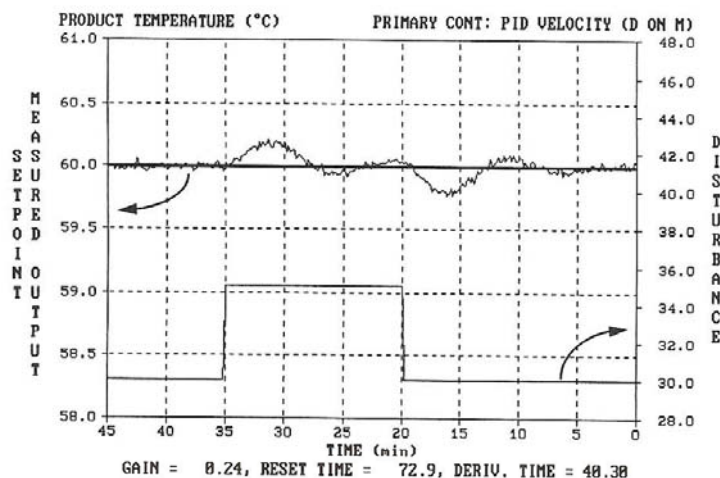


Figure 8 - Regulatory Performance of the Cascade Jacketed CSTR

disturbance variable rather than a secondary process output measurement), two algorithms (feed forward requires development of a disturbances-to-measured-output model combined with a feed back controller rather than two cascading feed back controllers) and one final control element.

Additional homework studies can focus on disturbances of different size, direction, shape or duration. The design objective can switch from disturbance rejection to set point tracking performance. A very challenging case study would be to focus on controller design at an *unstable, unsteady* state, such as 70 °C. Use your imagination to develop a variety of dynamics and control challenges using Picles. Needless to say, homework problems which begin "start with this transfer function and..." sound limiting indeed in comparison to the hands-on real world experiences possible with the Picles training simulator.

For More Information

For more information about Picles and available teaching materials, contact:

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(203) 486-4092
email: cooper@eng2.uconn.edu

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Acknowledgments

I would like to acknowledge my co-author, Jerry Bieszczad, for his efforts in Picles 4.0 development. As an undergraduate, Jerry's contributions were significant enough to earn him the position of top student architect. This achievement in no way diminishes the impressive contributions of my other student architects, without whom Picles would not exist. These include: Allen Houtz, Robert Schlegel (also contributing as an undergraduate) and Adam Lalonde.

The Right Tool for the Right Job - MathCAD in the Chemical Engineering Curriculum

By John Hwalek, University of Maine

Engineering educators have been encouraging students to use computers as problem solving tools for many years. Before user friendly programs such as spreadsheets became available, students had to solve problems by developing their own programs. In many cases, however, it was more expedient to solve a problem by hand due to the amount of time it took to develop the logic of a program and then debug and test it. Hence, the students' use of computers for problem solving was limited and occurred only when required.

The advent of easy-to-use, general purpose programs which have improved the computational power of the computer has, in turn, substantially increased the use of computers in problem solving. Spreadsheets, in particular, have made it easy to solve problems by setting up routines to do repetitive calculations or "what-if" analyses. Although not all problems can be easily solved using spreadsheets, many problems can be with little time needed for debugging.

Spreadsheets have improved problem solving capabilities; however, spreadsheets are not flexible because the solution is formatted in a rectangular form which is not ideal for many engineering problems. For many problems, the solution procedure must be transformed to fit the nature of the problem solving tool. Hence, it is often necessary to manipulate the program to obtain the desired result.

MathCAD, sold by MathSoft, Inc., is a computational tool which solves engineering problems efficiently and is currently being used in some classroom environments. Students have found the program not only easy to learn, but also useful for solving homework problems.

MathCAD's Capabilities

MathCAD may be best described as an "Engineering Spreadsheet". Similar to a spreadsheet, it is capable of substituting changes in variables into all predefined calculations and automatically recalculating corresponding values. The free format input and the WYSIWYG interface make MathCAD practical for use in engineering problems. MathCAD worksheets resemble scratch pads used to write down engineering equations and their calculated values. MathCAD's power, though, goes beyond simply plugging values into

equations. Some of MathCAD's additional features include:

- **Built-in dimensions and units.** The value for a dimensional variable is entered along with its units. MathCAD automatically converts units to base units and checks equations for dimensional consistency. Dimensional answers can be displayed in any units desired.
- **Built-in graphics.** Two- and three-dimensional plots can be easily created in the worksheet to display calculated results.
- **Non-linear equation solver.** MathCAD can automatically solve single or systems of non-linear equations numerically. The solution values can then be used in further calculations.
- **Numerical integration and differentiation.** MathCAD can numerically integrate and differentiate functions.
- **Vector and matrix calculations and functions.** MathCAD has built-in matrix and vector calculations and functions.
- **Complex numbers.** MathCAD can calculate expressions involving complex numbers including functions and numerical integration.

In addition, newer versions of MathCAD allow for symbolic calculations, transferring of information to and from other applications, and easy editing within the application.

Some of MathCAD's features which make the program well suited for chemical engineering calculations are demonstrated in Examples 1 and 2. In reading the examples note that expressions with a combined colon-equal sign ($:=$) indicate the assignment of a value to the variable on the left and that the equal sign by itself ($=$) indicates the value of the variable or expression on the left is being displayed.

Example 1 is a calculation of the convective heat transfer coefficient for benzene flowing in a pipe. This example demonstrates the ability of MathCAD to work with dimensional quantities using built-in units

conversion. Note that the defined variables have mixed units and that the result can be displayed in any units desired.

Example 2 is a calculation of the vapor-liquid equilibrium diagram for a mixture of hexane and heptane assuming an ideal mixture. Raoult's law is used along with Antoine's equation for the vapor pressures. This example demonstrates MathCAD's ability to solve non-linear equations and also the ability to plot calculated values. MathCAD uses "solve blocks" as a structure for numerically solving non-linear equations. An initial guess of the solution is required. The solve block structure starts with a *Given* statement and ends with a *Find*. Notice that the solution of Raoult's law to find the equilibrium temperature defines the temperature as a function of the liquid mole fraction $T(x)$. Each time $T(x)$ is to be evaluated, the solution of the non-linear equations inside of the solve block is found for the value of x defined by the function.

Integration of MathCAD into the Curriculum

MathCAD was integrated into the curriculum at the University of Maine when I introduced it to students in a junior level unit operations course five years ago. One lecture was spent demonstrating MathCAD capabilities and giving students a few instructions. It was then made available for students to use. As the semester progressed, the number of homework solutions being submitted with the calculations carried out using MathCAD increased. Faculty teaching other courses with these same students also found MathCAD being used to solve homework problems. It was observed that students were finally taking advantage of computers to solve problems in a natural way. The following year MathCAD was integrated into the department's first year computer course. Students throughout the curriculum now regularly use MathCAD to do calculations.

Use of MathCAD has allowed the assignment of more difficult problems. It has decreased the amount of time needed to set up and do calculations, leaving more time available to focus on the answer and its implications. Problems can be more design oriented with students carrying out what-if analyses by varying parameters. In some cases, students are required to develop the entire MathCAD solution on their own. For problems that are more complex, students are given an example solution which they are then able to modify. MathCAD has proven to be a much more successful teaching tool than FORTRAN. A major advantage of MathCAD is that the solution method is clearly presented in the worksheet. This is preferable to requiring students to modify programs in FORTRAN.

MathCAD has been used by students in several different courses at the University of Maine. In the second

year mass and energy balance course, it is used for routine calculations. In the process control course, it has been used to integrate differential equations for dynamic simulations as well as to construct Bode plots and Nyquist diagrams for design in the frequency domain. In the unit operations courses, it has been used for fluid flow and heat transfer calculations as well as for separations equipment design. In addition, programs have been developed to construct McCabe-Thiele diagrams as well as to do stage-by-stage solution of the MESH equations.

Although MathCAD is very versatile, there are problems for which other tools are better suited. In some ways, MathCAD is a black box. When the problem focuses on the details of the computational method, programming languages such as FORTRAN are more appropriate. Problems that are of a rectangular nature (e.g., cash flow calculations or flowsheet balances) are probably better solved using a spreadsheet. In spite of some of these shortcomings, MathCAD has proved to be a practical computer tool for students.

Forming a Chemical Engineering MathCAD Users Group

The reason for writing this article is to inform other chemical engineering educators of MathCAD and its capabilities. If your university is not using MathCAD or a similar program now, I recommend that you try MathCAD and make it available to students. If you are currently using this program in your curriculum, I am interested in knowing how it is being used in various courses. In addition, I am very interested in forming a Chemical Engineering MathCAD Users Group through which MathCAD worksheets could be shared and MathCAD topics, particularly related to pedagogical issues of using MathCAD, could be discussed. If there is enough interest, I will work on setting up a users group and possibly even an ftp site.

For more information or suggestions, please contact:

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University of Maine
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email: hwalek@maine.maine.edu

Platforms and Hardware/Software Requirement

MathCAD is available to run on IBM PCs and compatibles, Macs, and UNIX platforms. Some of the requirements are listed in Table 1.

References

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Table 1. MathCAD Platform and Hardware/Software Requirements

- IBM PCs and Compatibles
- MathCAD version 2.5 and below: 808x processor, DOS. Coprocessor not required.
- MathCAD version 3.1: 80286 + processor, Windows 3.1. Coprocessor not required.
- MathCAD version 4.0+: 80368 + processor, Windows 3.1. Coprocessor not required.
- Mac version: 68020+ processor
- UNIX Platforms
- MathCAD will run under UNIX on the following systems: DEC, HP, IBM RS/6000, Sun and Silicon Graphics.

Example 1: This program calculates the convective heat transfer coefficient for turbulent flow in a pipe.

Thermophysical properties of benzene

$$\mu := 1.16 \frac{\text{lb}}{\text{ft} \cdot \text{hr}} \quad \rho := 53.1 \frac{\text{lb}}{\text{ft}^3} \quad C_p := \frac{\text{BTU}}{\text{lb} \cdot \text{F}} \quad k := 0.089 \frac{\text{BTU}}{\text{hr} \cdot \text{ft} \cdot \text{F}}$$

Pipe dimensions (1 in Sch 40)

$$D := 1.049 \text{ in} \quad A := \frac{\pi}{4} D^2$$

Fluid flow rate

$$Q := 20 \frac{\text{gal}}{\text{min}} \quad v := \frac{Q}{A}$$

Calculate Re and Pr

$$\text{Re} := \frac{D \rho v}{\mu} \quad \text{Re} = 1.07 \cdot 10^5 \quad \text{Pr} := \frac{C_p \mu}{k} \quad \text{Pr} = 13.034$$

Calculate Nu

$$\text{Nu} := 0.023 \cdot \text{Re}^{0.8} \cdot \text{Pr}^{1/3}$$

Calculate heat transfer coefficient

$$h := \text{Nu} \frac{k}{D} \quad h = 581.533 \frac{\text{BTU}}{\text{hr} \cdot \text{ft}^2 \cdot \text{F}} \quad h = 3.302 \cdot 10^3 \frac{\text{W}}{\text{m}^2 \cdot \text{C}}$$

Example 2: This program calculates and plots an equilibrium diagram for an ideal mixture using Raoult's Law.

Antoine's coefficients for hexane (C6) and heptane (C7)

$$A_{C6} := 6.87776$$

$$B_{C6} := 1171.530$$

$$C_{C6} := 224.366$$

$$A_{C7} := 6.90240$$

$$B_{C7} := 1268.115$$

$$C_{C7} := 216.900$$

$$vp_{C6}(t) := 10^{A_{C6} - \frac{B_{C6}}{t + C_{C6}}}$$

$$vp_{C7}(t) := 10^{A_{C7} - \frac{B_{C7}}{t + C_{C7}}}$$

Set pressure (in mm Hg) Pt:=760

Find the boiling point T (in degrees C) for hexane and heptane

Guess Tb for hexane and heptane:

$$Tb_{C6} := 50$$

$$Tb_{C7} := 60$$

Given

$$vp_{C6}(Tb_{C6}) = Pt$$

$$Tb_{C6} := \text{Find}(Tb_{C6})$$

$$Tb_{C6} = 68.74$$

Given

$$vp_{C7}(Tb_{C7}) = Pt$$

$$Tb_{C7} := \text{Find}(Tb_{C7})$$

$$Tb_{C7} = 98.427$$

Solve for mixture boiling point temperature and vapor composition given total pressure and liquid composition. Assume Raoult's Law and Dalton's Law hold.

Initial guess of temperature for solve block:

$$Tb := \frac{Tb_{C6} + Tb_{C7}}{2}$$

Find mixture equilibrium temperature as a function of liquid mole fraction (x).

Given

$$x \cdot vp_{C6}(Tb) + (1-x) \cdot vp_{C7}(Tb) = Pt$$

$$T(x) := \text{Find}(Tb)$$

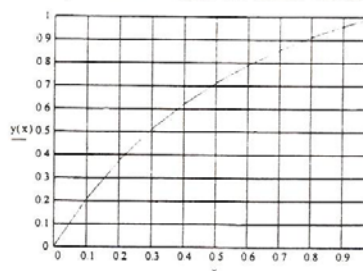
Define vapor mole fraction as a function of liquid mole fraction

$$y(x) := x \cdot \frac{vp_{C6}(T(x))}{Pt}$$

Plot equilibrium (x-y) diagram

x:=0.01..1.0

Equilibrium Diagram for hexane-heptane



ANNOUNCEMENTS

Election of CACHE Officers

CACHE is pleased to present the results of the July 15, 1994 officer elections. The offices of President, Vice-President, and Secretary will be as follows:

President

Warren D. Seider
University of Pennsylvania

Warren is Professor of Chemical Engineering at the University of Pennsylvania. He is an expert in process analysis, simulation, design and control; phase and chemical equilibria; azeotropic distillation; heat and power integration; and applied numerical methods.

A graduate of the Polytechnic Institute of Brooklyn and the University of Michigan, Warren joined the faculty of the University of Pennsylvania in 1967.

Warren teaches courses with emphasis on process design and control. He has co-authored *Introduction to Chemical Engineering and Computer Calculations* (with A. L. Myers) and *FLOWTRAN Simulation - An Introduction* (with J.D. Seader and A. C. Pauls). Warren helped to organize CACHE and served as the first chairman from 1971-1973.

In 1992, Warren was the recipient of the AIChE Computing in Chemical Engineering Award. A former AIChE Director, he has served the Institute in several capacities, including as chair and executive committee member of the CAST Division and as the 1991-1992 Publications Committee Chair.

Vice President

Lorenz T. Biegler, *Carnegie-Mellon University*

Lorenz T. (Larry) Biegler is currently professor of chemical engineering at Carnegie Mellon University, where he has worked since receiving his Ph.D. from the University of Wisconsin in 1981. His research interests are in the areas

of computer aided process analysis and design and include flowsheet optimization, optimization of systems of differential and algebraic equations, reactor network synthesis and algorithms for constrained, nonlinear process control.

Professor Biegler has been a visiting scholar at Northwestern University, a scientist-in-residence at Argonne National Lab and a Distinguished Faculty Visitor at the University of Alberta. He has authored or co-authored over 95 technical publications and presented numerous papers at national and international conferences. He received a Presidential Young Investigator Award from the National Science Foundation, is listed in *Who's Who in Science and Engineering* and *Who's Who in Engineering*. He has held several offices in the American Institute of Chemical Engineers and is also a member of SIAM, ACS and Sigma Xi. In addition, Professor Biegler has been an active consultant on process design and optimization strategies for the chemical and process industry.



Larry Biegler

Secretary

Jim F. Davis
Ohio State University

Jim Davis is a Professor of Chemical Engineering at Ohio State University and is also currently holding the position of Associate Director of Research Computing with Academic Technology Services. His early background was in control, modeling and simulation. Since the early 1980s, his primary research interests have been focused on Intelligent Systems in process and manufacturing operations. He came to Ohio State with industrial process operations experience through Amoco Chemicals Corporation and Argonne National Laboratory. Research work at OSU has led to the development of several programming approaches



Jim Davis

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for building intelligent systems and to the implementation of a number of integrated knowledge-based and neural network systems in a variety of industrial applications. He has consulted extensively in the area of applied expert systems and neural networks and has taught a number of industry-oriented short courses. In addition, he is involved in interdisciplinary research teams developing computer systems in manufacturing control, medicine, life-cycle design and high performance simulation. At Ohio State, he heads the AI in Chemical Engineering group within the Laboratory for AI Research (LAIR). He is a CACHE trustee and currently serves on the executive committee as secretary.

Monsanto Recognized for Aid to Education

In recognition of an unusual form of aid to education, Monsanto Co. was presented a plaque by the CACHE Corporation during the annual meeting of the American Institute of Chemical Engineers held in St. Louis, Nov. 6-12, 1993. The plaque was given to Monsanto "in appreciation for facilitating the introduction of computer-aided processing simulation, by means of FLOWTRAN, to the undergraduate chemical engineering curriculum".

In cooperation with CACHE Corporation, on Dec. 10, 1973, Monsanto announced that it would make its proprietary computer program FLOWTRAN (FLOWsheet TRANslator) available to universities for educational use.

FLOWTRAN permitted the steady state simulation of a large number of industrial processes. At the time, Monsanto loaned specialists from its Engineering Department and made a cash grant to help in the start-up of the computer programs.

FLOWTRAN was initially available over a time sharing system but in November 1983 Monsanto reiterated its support of chemical engineering education and allowed the distribution of FLOWTRAN to run on the universities' own computers. Since that time, the program has been distributed to 190 educational institutions worldwide, including 152 institutions in the United States and Canada.

FLOWTRAN has been used within Monsanto since 1966.

The alliance of chemical engineering educators who coordinated FLOWTRAN efforts at the university level was established by the National Academy of Engineering's Commission on Education as the CACHE (Computer Aids for Chemical Engineering Education) Committee. In 1975 it was formally organized as the CACHE Corporation, a not-for-profit entity. Professor Michael Cutlip of the University of Connecticut is its current president.

CACHE Process Design Case Study Volume 7

Process Integration of an Ethylene Plant



Monsanto Group Receiving CACHE Recognition for FLOWTRAN
AIChE Meeting, November 1993

Process integration (PI) technology refers to the chemical engineering principles and practice for systematically integrating the use of materials and energy in process plants. The technology was initiated in the late 1970's for more system-oriented and integrated approaches in process plant design and retrofit for saving energy and increasing profits, and an important early development was the pinch design method for heat-exchanger networks (HENs). Significant advances of the PI technology in the 1990's have greatly broadened its applications to include emission control, waste reduction and

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wastewater minimization, etc. In a September 1992 article, entitled "Use Process Integration to Improve Process Designs and the Design Process," appearing in Chemical Engineering Progress, Steve Morgan states that: "At the M. W. Kellogg Co., we firmly believe that PI technology is just good process design and every process engineer should understand and know how to use these tools."

This case study teaches the reader how to carry out the improved design of an ethylene plant using two commercial process-integration software tools, ADVENT by Aspen Technology, Inc. (Cambridge, MA) and SUPERTARGET by Linnhoff March, Inc. (Houston, TX and Manchester, UK) that are readily available to academic users at low costs. The original problem definition came from the EXXON Corporation and the results of an earlier CACHE Process Design Case Study of the same problem were published as Volume 1 in 1985. The process consists of a gas-compression train and a separation train only. Crackers, furnaces and the preliminary gas-fractionating column do not appear in the flowsheet.

The specific tasks of this case study are: (1) to introduce practical guidelines for extracting data for process and utility streams and for refrigeration cycles, to facilitate their use in process integration; (2) to identify useful heuristics for specific process-integration activities, such as heat integration, utility placement and refrigeration selection, and to provide physical and graphical explanations of the results of these activities; and (3) to develop better retrofit

and grassroots designs of the HEN and refrigeration system in the CACHE ethylene plant (Volume 1) and investigate the merits of the designs in terms of payback time and total annualized cost.

Because the costing methods used in the earlier CACHE report are impractical for computerized implementation with ADVENT or SUPERTARGET, this case study devises its own cost laws and evaluates various design options by its own costing basis. In particular, this case study considers the HEN and refrigeration system in the CACHE design, discusses the options for retrofitting this design and gives two cheaper grassroots designs: one at a minimum-approach temperature (MAT) of 10°C and one at a MAT of 2.5°C. This study finds that automated MAT optimization may not properly indicate the possibilities for cost reduction when different utility mixes are available for optimal utility placement and refrigeration selection at different MATs.

This case study has been prepared by Gert-Jan (John) A. F. Fien and Y. A. Liu, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061-0211, with financial support from the National Science Foundation, Division of Engineering Education and Centers, through the SUCCEED Center of Excellence in Undergraduate Engineering Design at Virginia Tech.

To order a copy of the CACHE Process Design Case Study - Process Integration of an Ethylene Plant, please complete the order form below.

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