CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 44 SPRING 1997

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 (Computer Aids 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:

CACHE Corporation
P. O. Box 7939
Austin, Texas 78713-7939
(512) 471-4933
FAX: (512) 295-4498
cache@uts.cc.utexas.edu

http://www.che.utexas.edu/cache

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 Christine Bailor with contributions from a number of CACHE members and representatives.

CACHE NEWS

No. 44 **Spring 1997**

CACHE Trustees

President
Lorenz T. Biegler, Carnegie Mellon University
(biegler@cmu.edu)

Vice President
James F. Davis, Ohio State University
(davis@kcgl1.eng.ohio-state.edu)

Secretary
Andrew N. Hrymak, McMaster University
(hrymak@mcmaster.ca)

Executive Officer
David M. Himmelblau, University of Texas at Austin
(himmelblau@che.utexas.edu)

Academic Trustees
Brice Carnahan, University of Michigan
(carnahan@engin.umich.edu)
Peter Cummings, University of Tennessee
(ptc@utk.edu)
Michael B. Cutlip, University of Connecticut
(mcutlip@uconnvm.uconn.edu)
Michael F. Doherty, University of Massachusetts
(mdoherty@ecs.umass.edu)
Thomas F. Edgar, University of Texas at Austin
(edgar@che.utexas.edu)
H. Scott Fogler, University of Michigan
(sfogler@engin.umich.edu)
Ignacio Grossmann, Carnegie Mellon University
(grossman@cmu.edu)
Sangtae Kim, University of Wisconsin
(kim@chewi.che.wisc.edu)

Academic Trustees
Manfred Morari, ETH Zurich
(morari@aut.ee.ethz.ch)
Gintaras V. Reklaitis, Purdue University
(reklaiti@ecn.purdue.edu)
Peter R. Rony, Virginia Polytechnic Inst. and State Univ.
(rony@vt.edu)
J. D. Seader, University of Utah
(seader@ute.cc.utah.edu)
Warren D. Seider, University of Pennsylvania
(seider@cheme.seas.upenn.edu)
George Stephanopoulos, Massachusetts Inst. of Tech.
(geosteph@mit.edu)
Ross Taylor, Clarkson University
(taylor@sun.soe.clarkson.edu)
Venkat Venkatasubramanian, Purdue University
(venkat@ecn.purdue.edu)

Industrial Trustees
Rakesh Agrawal, Air Products and Chemicals
Joseph Boston, Aspen Technology
(boston@aspentec.com)
Ferhan Kayihan, IETek, Integrated Engr. Tech.
(fkayihan_ietek@msn.com)
Edward M. Rosen, EMR Technology Group
(73141.3376@compuserve.com)
Jeffrey J. Siirola, Eastman Chemical Company
(siirola@eastman.com)
David Smith, E.I. DuPont de Nemours & Co. Inc.
(wdsmith@esspt0.dnet.dupont.com)
Joseph D. Wright, Pulp and Paper Research Inst. Canada
(wright@paprican.ca)

CACHE Task Forces and Committees

Standing Committees

Publications
Prof. Brice Carnahan
Dept. of Chemical Engineering
University of Michigan
Ann Arbor, Michigan 48109
(313) 764-3366

Newsletter
Prof. David M. Himmelblau
Dept. of Chemical Engineering
University of Texas at Austin
Austin, Texas 78712
(512) 471-7445

Development
Prof. Thomas F. Edgar
Dept. of Chemical Engineering
University of Texas at Austin
Austin, Texas 78712
(512) 471-3080

Conferences
Dr. Jeffrey J. Siirola
Eastman Chemical Company - B95
P.O. Box 1972
Kingsport, TN 37662-5150
(423) 229-3069

Task Forces

Artificial Intelligence
Prof. George Stephanopoulos
Dept. of Chemical Engineering
Massachusetts Institute of Technology
66-444
Cambridge, Massachusetts 02139
(617) 253-3904

Process Engineering
Dr. Edward M. Rosen
EMR Technology Group
13022 Musket Ct..
St. Louis, Missouri 63146
(314) 434-5498

Case Studies
Prof. Manfred Morari
Automatic Control Lab
ETH/Zentrum/ETL 129
Zurich CH-8092
Switzerland
41 1 632 7626

CD Development
Prof. Peter Rony
Dept. of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, Virginia 24061
(703) 231-7658

Curriculum
Prof. James F. Davis
Dept. of Chemical Engineering
Ohio State University
140 West 19th Avenue
Columbus, OH 43210-1180
(614) 292-0090

Molecular Modeling
Prof. Peter Cummings
Dept. of Chemical Engineering
University of Tennessee
419 Dougherty Hall
Knoxville, TN 37996-2200
(703) 231-7658

NSF Development of Innovative Engineers
Prof. H. Scott Fogler
Dept. of Chemical Engineering
3168 Dow Building
University of Michigan
Ann Arbor, Michigan 48109
(313) 763-1361

NSF Simulated Laboratory Modules
Prof. Gintaras V. Reklaitis
School of Chemical Engineering
Purdue University
West Lafayette, Indiana 47907
(317) 494-4075

Internet 2

Tom Edgar, University of Texas
and Jim Davis, Ohio State University

Nearly 100 US. research universities have joined to participate in the creation of a new national network, called Internet 2 (I2), that is dedicated to research and education. I2 will be a nationally coordinated network architecture that will offer vastly higher connection speeds and more reliable service. The larger "pipeline" — 100 to 1000 times faster than today's Internet — will allow the simultaneous transmission of voice, video, and data to enable distance learning, enhance digital libraries, and make possible new realms of on-line collaborative research. Such a network can transmit the contents of the entire Encyclopedia Britannica in under a second.

Today's Internet represents the largest change in human communications since the printing press. Every day, this rapidly growing global network touches the lives of millions of Americans. Students log in to the Library of Congress or take virtual field trips to the archeological sites. Entrepreneurs get the information they need to start a new business and sell their products in overseas markets. The Internet is a commercial outgrowth of federal investment in research networks. President Clinton's recently announced "Next Generation Internet" initiative intends to continue national investment with proposed funding of $100 million per year and connect universities and national labs with high-speed networks.

Higher-speed, more advanced networks will enable a new generation of applications that support multimedia, scientific research, national security, distance education, and health care. For example, Universities are now piloting near term technologies such as two-way video to remote desktops. VCR-like replay of past lectures, modeling and simulation, collaborative environments, and on-line access to courseware, i.e., instructional software. Distance education will improve the ability of universities to serve working Americans who want new skills, but who cannot attend a class at a fixed time and place during the week.

The charter university members have agreed to establish and finance a new organization to help create the network. This university consortium, together with a number of federal research and development agencies — the National Science Foundation, the Advanced Research Projects Agency, the Department of Energy, NASA, and the National Institutes of Health — and leading computer and telecommunications firms, will not only design and develop the network, but will develop applications for its use, and will rapidly disseminate the fruits of their research and development to the broader Internet community.

The universities who make up the Internet 2 consortium hope to have the first connections running in six months. Academic representatives met in San Francisco earlier this year to discuss technical issues and lay the groundwork for the future. Universities are excited by the prospect of a system that would let researchers develop new tools similar to the innovation of the World-Wide Web. A number of member colleges and universities have already made commitments to another effort, the Very High Speed Backbone Network Service, or vBNS, run by the National Science Foundation that will likely be integrated with I2.

Internet 2 will rely on participants' joining forces in various multistate regions of the country to build extremely high-speed regional networks. Each of these shared pieces of the Internet 2 infrastructure would be known as a "gigapop," which stands for "gigabit capacity point of presence." A gigabit connection can offer speeds hundreds of times as fast as today's typical Internet connection. In addition to contributing to the development of regional gigapops, participants must pay for a high-speed connection between the gigapop and campus networks and improve the speed of connections all the way down to the desktop computers of the campus users. There may be as many as 30 gigapops established in the United States over the next three to five years.

The CACHE Molecular Modeling Task Force

Peter T. Cummings
University of Tennessee and Oak Ridge National Laboratory

Introduction

It is my privilege to have recently been elected a Trustee of the CACHE Corporation, and I was asked to describe what I expected my activities as a CACHE Trustee would involve. In this brief article, I will attempt to do just that.

Most of my activities will revolve around the CACHE Molecular Modeling Task Force (MMTF) established in 1996. In addition to myself, the MMTF consists of task force co-chair Warren Seider (University of Pennsylvania), Arup Chakraborty (University of California Berkeley), Ariel Chialvo (University of Tennessee), Hank Cochran (Oak Ridge National Laboratory), Juan de Pablo (University of Wisconsin), David Kofke (SUNY Buffalo), Edward Maginn (University of Notre Dame), Thanasis Panagiotopoulos (Cornell University), Richard Rowley (Brigham Young University), Randy Snurr (Northwestern University) and Phil Westmoreland (University of Massachusetts). During his sabbatical at Cornell University, Nigel Seaton (Cambridge University) is also participating in the task force. Each participant in the MMTF has a strong interest in and commitment to education as well as a successful research program in molecular modeling. The term "molecular modeling" encompasses those emerging computational techniques that explicitly use a molecular-based approach to address problems of importance in chemical engineering. These include molecular simulation techniques such as molecular dynamics and Monte Carlo calculations and related techniques. A second area of focus is computational chemistry centered on applied quantum mechanics which predicts molecular structures and force fields. Molecular-based theoretical methods complement simulation and computational chemistry, unifying the body of computational results and providing entry to problems currently beyond their reach.

The MMTF came into existence largely at the urging of Warren Seider who, during his tenure as CACHE President, participated in the Seventh International Conference on Fluid Properties and Phase Equilibrium for Chemical Process Design in Snowmass, CO, in 1995. At that meeting, Thanasis Panagiotopoulos and I presented workshops on Monte Carlo simulation and molecular dynamics simulation respectively which were heavily attended both by academic and industrial participants. The popularity of these workshops prompted Warren to initiate the establishment of the MMTF as an activity within CACHE. As a non-profit corporation which is devoted to the development of computer-based educational aids for chemical engineering, and which has demonstrated considerable foresight in the past by brokering the introduction of computer-aided process flowsheeting to the undergraduate chemical engineering curriculum, CACHE can play a significant and unique role in bringing instruction in molecular methods into the chemical engineering classroom. We believe that the timing for such an initiative could not be better: driven by unprecedented exponential growth in computing power, computational molecular-based technologies are making significant inroads in industry, so that the demand for knowledge in these areas by chemical engineers will increase dramatically over the next few years. By fostering the development of educational materials and technologies to serve this growing need, we hope that CACHE can repeat its great success in bringing computer-aided process design methods to the classroom for the new generation of computer-aided molecular product design methods.

Molecular Modeling Task Force Activities

The growth of the industrial usage of molecular simulation and quantum mechanical methods implies that all chemical engineers will require familiarity with these methods, just as industry assumes chemical engineers will be familiar with process flowsheeting packages today. Molecular modeling methods can and will appear in undergraduate curricula in several ways: as segments of existing core undergraduate courses (for example, Thermodynamics, Kinetics, Transport and Design courses, in the latter case as molecular product design); within elective courses (for example, Biochemical Engineering and Materials Science); and as dedicated courses. Several chemical engineering departments already have undergraduate courses which involve molecular modeling methods. Examples of dedicated courses include: at the University of Pennsylvania, *Advanced Thermodynamics* is a required course that involves molecular simulation, particularly Monte Carlo; MIT offers an elective on *Applied Quantum Mechanics*; and at the University of Wisconsin, the Chemistry and Chemical Engineering departments alternate teaching *Advanced Physical Chemistry* which involves statistical mechanics and quantum mechanics. To ensure that molecular modeling methods enter the undergraduate curriculum in a smooth and useful way, textbook and sample program materials need to be

developed that can be used by non-experts in the field. The goal of the CACHE MMTF is to play a major leadership role in the development of these course materials. It can also serve as the focal point for training of chemical engineering faculty in this area.

There are two principal curriculum-related activities planned for the CACHE MMTF: The first activity is the development of a World Wide Web (WWW)-based textbook on molecular simulation which could serve as the primary textbook for a graduate level course on molecular modeling, or as a secondary resource in undergraduate thermodynamics courses. The second activity is the development of educational modules in molecular modeling which can be used in several courses in the undergraduate chemical engineering curriculum to illustrate the use of molecular concepts and molecular modeling tools.

WWW-Based Textbook on Molecular Simulation. The first activity of the MMTF is the development of WWW-based textbook on molecular simulation. The core of the text will contain expositions of the basic elements of molecular simulation, covering theoretical and practical aspects of the craft. Supplementing this will be a set of review chapters providing in-depth coverage of various simulation techniques; many of these chapters will be authored by specialists that have committed to the project. (See Table I.) Also, we plan to incorporate "case studies", special sections that expand on *significant* advances in the peer-reviewed literature. Such material will be prepared by the article's author, and will allow him or her to elaborate on the topic, unhindered by the confines of the standard journal article; thus he or she will perhaps supply examples, data, programming code or other information enabled by the WWW medium. Finally, instructors using the text for a class will be requested to submit contributions, which would typically take the form of solved "homework" problems, teaching supplements, or interesting sidelights of simulation methodology; contributions might even be generated by students assigned semester projects that require creation of a hypertext document for inclusion in the text. All contributions will be rigorously reviewed to ensure adherence to the highest standards of science and pedagogy. The review will be overseen by a broad panel of experts in molecular simulation. Some of these persons are listed in Table I; as the project develops, we will solicit contributions or reviews from specialists with expertise in areas not represented in our initial panel. This project is being funded by a $346,000 grant from the Combined Research and Curriculum Development program of the National Science Foundation for the period April 1, 1997-March 30, 2000.

Table I. Participants in the WWW-based text project.

Contributor	Specialty/Interests in Molecular Simulation
P. T. Cummings	molecular dynamics; parallel computation; intermolecular potentials; supercritical fluids
D. A. Kofke	Phase equilibria; solids; mixtures; liquid crystals; intermolecular potentials
H. D. Cochran	solution thermodynamics; molecular dynamics; parallel computation
J. J. de Pablo	polymer solutions, melts, and solids; parallel computation
D. J. Evans	molecular dynamics, particularly non-equilibrium; transport properties
A. Z. Panagiotopoulos	polar and ionic fluids; surfactants; polymers; intermolecular potentials; critical phenomena
R. L. Rowley	molecular dynamics, non-equilibrium molecular dynamics, transport properties, and mixture properties

Development of Educational Modules in Molecular Modeling. One of the primary goals of the MMTF is to provide a unifying organization and framework for the development of educational modules for incorporation into undergraduate and graduate chemical engineering curricula and for use in continuing education. To ensure maximum accessibility and platform independence, the preferred environment for educational module development will be the World Wide Web. The emerging Java programming language standard will enable the development of interactive pages with sophisticated graphics and animation capabilities. Support for this project will be sought by submitting a curriculum development proposal to the National Science Foundation with support from the CACHE Corporation. Selected examples of modules that have been

suggested for development are given below, organized by subject area.

In **thermodynamics**, molecular modeling modules can be produced that would allow students to study the relationship between chemical constituency and macroscopic thermodynamic properties. For example, modules permitting observation of fluid properties as molecular structure and intermolecular potentials are independently changed would help students to develop a feel for what to expect of previously unencountered chemicals and their mixtures. **Transport and separation processes** are ultimately molecular processes. Thus, transport courses, and unit operations courses which incorporate transport and separations, offer tremendous opportunities to demonstrate the phenomena at a molecular level. Modules illustrating diffusion, viscosity, thermal conductivity, adsorption and diffusion in membranes are planned. Many additional modules are possible, including modules demonstrating vapor-liquid equilibrium by Gibbs ensemble Monte Carlo simulation, molecular-level simulation of lubrication, and molecular-level processes in stick and slip boundary conditions.

Chemical reactions occur because of molecular events, so the study of **chemical reaction kinetics** provides ample opportunities for approaching the phenomena on a molecular scale. Molecular modeling methods can be particularly useful in explaining concepts of heterogeneous catalysis and transport in porous catalytic materials. The literal explosion in the application of molecular modeling methods to biological systems means that modules can be developed which demonstrate the molecular basis for many important biological processes studied in **biochemical engineering**, such as the diffusion of ligands and their binding to cell receptors, the folding of proteins into specific function forms and adsorption of biomolecules on surfaces.

In addition to curriculum activities, the MMTF will concern itself with several activities designed to further the scope and application of molecular modeling methods in chemical engineering. Based on the highly successful FOCAP format used by other task forces in CACHE, we hope to establish a new triennial conference "Foundations of Molecular Modeling." The target audience for the conference will be practitioners (both in industry and academia), those interested in becoming practitioners (both in industry and academia), and those involved with industrial managers who wish to learn about the technology. The target first year for the conference will be 2000 and will be promoted as FOMM 2000. The funding mechanism for FOMM 2000 and beyond will follow the FOCAP model: Several divisions of the National Science Foundation (such as Chemical and Thermal Systems and Materials Research) and industrial sponsors would be approached to fund part of the expenses of the conference. The remainder of the conference expenses would be funded by registration fees.

As well as the FOMM 2000 activity, the MMTF members are committed to providing tutorials on molecular modeling methods in two main formats: short (2-3 hour) introductory tutorials and longer, multi-day short courses. The primary target audience for the introductory tutorials will be industrial managers and researchers, and academic researchers (faculty or graduate students) unfamiliar with molecular tools. The objective of the introductory tutorials will be to give the participants sufficient information to decide whether they would like to invest more time and effort to go into more depth into the subject. Opportunities for the introductory tutorials are provided by the spring and/or fall national AIChE meetings and will be coordinated with the existing programming activities of the AIChE.

The multi-day short courses would involve hands-on experience, and the participants would be expected to leave with a demonstrable skill in molecular modeling. Public domain software will be used in the courses. The courses will be held in conjunction with conferences, such as FOMM 2000. The target audience will be industrial and academic "committed beginner" researchers in the area. Some of the material will be of advanced nature, but most would be at an introductory level. An additional avenue for such a short course may be the AIChE Continuing Education program.

A related, specific initiative for the MMTF was to propose to the AIChE that a topical conference on molecular modeling and computational chemistry. This topical conference has now been approved by the AIChE and will be held at the 1998 annual (fall) meeting in Miami Beach. Phil Westmoreland, Ken Cox and I will be the conference co-chairs.

Conclusion

The next few years will be busy ones for the MMTF. I look forward to the continuing very productive association with CACHE as we move towards fulfilling the goals of the MMTF.

Acknowledgments

Much of the text given above describing the planned and current activities of the MMTF was developed jointly with the MMTF members. In particular, I am indebted to my colleague David Kofke (SUNY-Buffalo) who, while in sabbatical at the University of Tennessee during the 1996-97 academic year, has been an invaluable contributor to the efforts of the MMTF.

The "Chicago" CD-ROM
AIChE/CACHE Meeting

Peter R. Rony
Virginia Polytechnic Institute & State University

Introduction

When he became chairman of CACHE several years ago, Mike Cutlip's vision about his proposed CD-ROM initiative had several elements:

(1) Provide a CACHE CD-ROM "deliverable" to CACHE-member chemical engineering departments, as well as to both ChE students and faculty.

(2) Provide ChE students directly with a CACHE deliverable, rather than indirectly through ChE faculty.

(3) Demonstrate the value of CD-ROM technology to the AIChE as a possible replacement for their extended abstracts booklet.

With the successful completion of the "Chicago CD-ROM disc", all three elements of Mike's vision have been accomplished. Elements (1) and (2) were accomplished with the Volume 1 (November 1994) and Volume 2 (April 1996) CACHE CD-ROMs, and element (3) was accomplished at the Chicago AIChE annual meeting with the "Chicago" CD-ROM (November 1996).

The primary objective of the "Chicago" CD-ROM disc developed under a collaborative arrangement between AIChE headquarters and the CACHE Corporation was to provide an electronic substitute for the "Extended Abstracts" volume that contained printed versions of the abstracts for every presentation in every session at the AIChE Annual Meeting. The printed version costs $50,000, a sum that may not even include the value of the time of the professionals who put it together. The electronic extended abstracts, namely, the "Chicago" CD-ROM disc costs substantially less to produce.

The" Chicago" CD-ROM disc was an AIChE experiment in electronic information transmission. The heart of the CD-ROM was a faithful subdirectory-and-file reproduction of the AIChE Chicago abstracts web site created by Dale Kirmse at the University of Florida. The last electronic "draft" of the 2701-file hierarchical subdirectory ^ consisting of subdirectories \sessions, \particip, \sessions\by_time, \sessions\by_area, and \area10b — was transmitted from Dale to the CD-ROM editor by October 2, 1996. This transmission "fixed" the web site on the ensuing "Chicago" CD-ROM that meeting participants purchased for $25 (ChE professionals) or $15 (ChE students).

Just as was the case with the creation (during the late 1980s) of CAST Communications the newsletter of the AIChE Communications and System Technology division — it required a triumvirate to produce the "Chicago" CD-ROM. Sangtae Kim (University of Wisconsin), as meeting program chairman (MPC) for the Chicago Annual Meeting had the vision and guts to go ahead with the project, obtain funding, convince AIChE headquarters, and solve numerous abstract acquisition problems; Dale Kirmse (University of Florida) created the "Chicago" meeting AIChE World Wide Web site, made certain that all the links operated correctly, and compressed it as several *.ZIP files that were available at a UFlorida FTP site; and finally, Peter Rony (Virginia Tech) acquired via FTP the *.ZIP files and wrote them to a master CD-R disc to which he added both a "Chicago" graphical user interface (GUI) called CHICIVW4.EXE and an abbreviated version of the Volume 2 CACHE CD-ROM. With computer projects in ChE, it seems not to take "a village," but rather, "a triumvirate."

The Four CD-ROM Project Stages

The "Chicago" CD-ROM project had four development stages:

Stage One: (a) The decision to create a "Chicago" CD-ROM; (b) The announcement of the CD-ROM; (c) The acquisition of paper abstracts for the University of Florida AIChE WWW site maintained by Dale Kirmse.

Stage Two: (a) The creation of a robust "Chicago" annual meeting web site at the University of Florida server maintained by Dale Kirmse. [NOTE: By robust, it is meant that all the WWW links worked correctly.]

Stage Three: (a) The transfer of the "Chicago" subdirectories and HTML files from the University of Florida to Peter Rony in Blacksburg; (b) The transfer of these subdirectories and files to a write-once CD-ROM disc; (c) The replication of the master CD-ROM disc by a corporate replicator — in this case, Imation, Inc. (formerly a 3M division) — in Menomenie, Wisconsin; (d) The transfer of 1000 "Chicago" CD-ROMs, November 1996 annual meeting week.

Stage Four: (a) The publicizing, marketing, distribution, and sale of the 1000 CD-ROM discs by the AIChE staff at the Palmer House Hilton; (b) The continued sale and mailing, by

AIChE headquarters in New York, of any discs that remained unsold by the end of the Chicago meeting.

In his November 1996 CD-ROM Task Force report to the CACHE Trustees, the CD-ROM editor made the following points, some of which might be of interest to ChE colleagues who contemplate a CD-ROM project:

Will there be a Volume 3 CACHE CD-ROM in the Near Future?

No.

Why Not?

1996-97 is not a good time to tackle ambitious, multi-file, multi-subdirectory, multimedia CD-ROM projects because the Windows 95 platform still has software bugs and because the new Win32 applications also have software bugs. Even the new "plug-and-play" computer hardware has bugs when operated under Windows 95. Furthermore, we are in transition from the Windows 3.11 platform to Windows 95 platform. A developer cannot assume that all users employ Windows 95; he must develop software for the lowest-level platform, namely Windows 3.11 with the hope that it also will operate well on Windows 95. The CD-ROM editor has one remaining Windows 3.11 system left, his laptop PC; all other possible development systems have been converted to Windows 95. CD-ROM development had become a hassle in late 1996; more time is spent circumventing hardware and software bugs than actually accomplishing productive work on the CD-ROM GUI and its subdirectories and files. Perhaps Windows NT is a more robust programming platform.

The Browser Problem

Paul Rony (B.S. EE, VaTech, ,89), the son of the editor, used a "clean machine" to beta test the "Chicago" CD-ROM after the deadline for replication had passed. The surprise was that only IVIEW 2.0, of four possible "local" browsers, worked with Dale Kirmse's WWW files on the CD-ROM disc. Further, it was not practical to use Winzip 95 to decompress Dale's *.ZIP files; one had to resort to use WinZip 5.6 on Windows 3.11 to accomplish the task properly. With Winzip 95, any file called INDEX.HTM became INDEX~1.HTM, thus destroying every one of Dale's links.

The Platform Problem

During the late1960s, the typical computer was an IBM mainframe housed in an air-conditioned room with a window through which computer users submitted punched cards. Of interest is not the computer RAM, the processor speed, or the storage capacity, but rather the number of professionals who serviced the computer and interacted with users. A typical computer center usually had a minimum of 3 professionals and perhaps as many as 10-15 professionals associated with it. Fast forward to 1996, where computer hardware fully the computational equivalent (or superior) of a 1960s mainframe sits on a professional's desktop. Also, in 1996 we have a significant nuisance, computer viruses, which did not exist during the 1960s. One can ask: Where is the computer center? If the professional who uses this 1996-vintage desktop computer would look in a mirror, he would see the computer center himself. This transition from a multi-person to a "single-person computer center" has occurred in stages assembly language, DOS, Windows 3.1, and finally Windows 95 — so gentle that many of us have not realized what has happened to computing in the mid-1990s. The bugs and incompatibility problems associated with mid-1990s hardware and software can be simply overwhelming and completely detrimental to the task at hand viz., finishing a computer software project.

Abbreviated Volume 2 "Bonus" on Chicago CD-ROM Disc

The Chicago meeting CD-ROM disc contained a graphical user interface, CACHE12.EXE, that was an abbreviated version of the Volume 2 CACHE CD-ROM (which was distributed to ChE students and faculty during April 1996). This GUI contained the following menu categories: CACHE, AICHE, Demos, HTML, PDF, SciViz, and WWW. The 2D and 3D scientific visualization tutorial (see SciViz menu) was hoped to be of particular interest to users of the Chicago CD-ROM. There were also (1) tutorials on multimedia authoring (see Readme menu) and Windows-based Internet clients (see WWW and PDF menus); (2) AIChE membership documents (see AIChE menu) and corporate software demos and web presentations (see Demos and HTML); and (3) example images from CACHE educational software (see CACHE menu). At least 371 megabytes on the Chicago CD-ROM were associated with program CACHE12.EXE.

CD-ROM Statistics

Totals for the Chicago CD-ROM: 397,755,243 bytes in 7541 files contained within 3295 subdirectories.

Totals for the Chicago 1996 WWW files: 19,872,916 bytes in 2880 files contained within 2631 subdirectories.

CHICIVW4.EXE graphical user interface file: 3,203,427 bytes.

CHICNET6.EXE graphical user interface file: 3,375,316 bytes.

CACH12.EXE graphical user interface file: 15,285,336 bytes.

Totals for the abbreviated Volume 2 CACHE CD-ROM on the Chicago CD-ROM disc: 371,303,584 bytes in 4659 files contained within 664 subdirectories.

A Retrospective from the Year, 2006: The "Chicago" CD-ROM Project

Just how might history record the "Chicago" CD-ROM project during 1996? The editor suggests the following conclusions:

1. By Thursday afternoon, November 14, 1996, of the Chicago annual AIChE meeting, the CD-ROM project could fairly be judged as being successful — a conclusion based upon the number of sales of discs up to that day. Not a resounding success, but successful. Four full boxes of 1000 CD-ROM discs remained at the service center, which meant that almost 600 discs were sold, most at a price of $25 per disc.

2. Stage One, Stage Two, and Stage Three could be considered as all being successful. Stage Four was the weak link in the entire project.

3. The advertising metaphor used for the "Chicago CD-ROM" was probably inappropriate. It was the "A-B-C building-block metaphor." CD-ROM discs are round; blocks are square. A more appropriate advertising metaphor would have been something round — e.g., a plate, a disc, or a Frisbee. Perhaps the metaphor could have been a Frisbee sailing (not cruising) over the "information superhighway".

4. During Stage Four, we failed to provide a gentle transition for those colleagues who were more accustomed to the paper-based extended abstracts. We failed to rent and provide a group of personal computers and associated laser printers that would permit attendees to generate paper copies directly from CD-ROM discs. This would have been a powerful advertising mechanism — had it been used — to promote sales of CD-ROM discs. For example, the service center could have pointed out, "See how easy it is to generate printed copies, on a need-to-use basis, of precisely those presentations that you wish to attend."

5. Viewed from the year, 2006, we still have failed to produce at least ONE, ARCHIVAL PAPER COPY — at AIChE headquarters in New York — of the Chicago 1996 annual meeting. By 2006, CD-ROM optical technology is already obsolete, having been replaced by holographic crystals capable of storing up to 1 terabit of information in one cubic inch of material. Sure, we have a bunch of CD-ROM disc archives for the years 1996 through 2002, but there is not a single CD-ROM player, and associated software, remaining at AIChE headquarters. Further, AIChE headquarters failed to transfer the 1996-2002 CD-ROM discs to holographic crystals for archival purposes.

6. The typical "modest" 1996 "Chicago" CD-ROM web page contained no color image, no equation, no audio, no animation, and no video data types. The one-thousand-seven-hundred INDEX.HTM files contained only the "text" data type. One exception to this rule was CAST Area 10b, which used PostScript or encapsulated PostScript. Nobody from Area 10b ever explained to the Stage 3 developer why Adobe Acrobat PDF files were not used instead of raw, unadulterated PostScript files.

7. The "Chicago" CD-ROM meeting abstracts comprised a total of approximately 20 megabytes. The marketing of the CD-ROM failed to mention that there were 371 megabytes of subdirectories and files — an abbreviated version of the Volume 2 CACHE CD-ROM — on the Chicago CD-ROM disc. The GUI that coordinated these subdirectories and files was known as CACHE12. EXE (Authorware 3.5); it contained audio, animation, and color image data files in abundance. The reason that this "bonus," as it was called in 1996 was not advertised was because the exact extent and nature of the bonus was finalized only during October 1996, approximately one month before the annual meeting. Advertising could not have been expected to announce the bonus in the meeting program; however, the meeting marketing group could have announced the bonus more publicly on the fourth floor registration area at the Palmer House.

8. The coordination between Stage 3 and Stage 4 was deficient. This fact was as much the fault of the Stage 3 developer as it was the Stage 4 personnel. The editor had a clear idea of what was likely to appear on the Chicago CD-ROM. No mechanism existed for him to communicate such information — including last minute omissions — to an individual at AIChE headquarters who was responsible for the CD-ROM visual publicity at the Palmer House Hilton registration area.

9. In retrospect, during most of the Chicago meeting it was not abundantly clear where one would purchase the Chicago CD-ROM within the fourth-floor registration area. The dominant message within the service center was "T-shirts." The visual advertising metaphor was blocks and squares, not discs and circles.

10. The fact that only approximately 600 CD-ROM discs were sold at the Chicago meeting can be viewed, in 2006, as a net loss of information transmission to attendees at the meeting. During the Miami Beach annual meeting in 1995, every participant went home with a heavy, thick, paper extended abstracts volume.

11. The 1996 Chicago annual meeting can be viewed, in 2006, as a year of transition and uncertainty concerning the issue of the preferred medium for abstracts — (a) an extended abstracts printed-paper volume for each participant, (b) the World Wide Web AIChE site, (c) a CD-ROM disc with no printing capability at the meeting site, or (d) an ability for attendees to view and print abstracts in the registration area [with an option to purchase the full CD-ROM]. At the time, the editor believed that the most appropriate strategy for the transition period was alternative (d).

ChemSep Case Book Supplemental

Ross Taylor
Clarkson University

For the past 8 years during fall semesters I have taught a junior/senior 3 credit course on mass transfer and stagewise operations. For the past several years I have made extensive use of ***ChemSep*** in this course for project work. In addition, ***ChemSep*** is used for many other exercises including the almost weekly Pepsi Challenge in which the class repairs to a computer laboratory where they conduct small scale design or simulation problems in a limited time (the one hour scheduled for the class). The students turn in their results at the end of the class, but are expected to finish their work before the next class period in the event that they did not complete the exercise. The first technically competent solution wins a Pepsi for those student(s). With this article we begin an occasional series that presents some of these problems with possible solutions.

1996 Pepsi Challenge
Round 6 - Azeotropic Distillation

Azeotropic distillation columns are among some of the most interesting to simulate; here we investigate the well known problem of separating ethanol(1) from water(3) using benzene(2) as an entrainer. These columns are interesting if for no other reason than that they can exhibit multiplicity. The purpose of this challenge problem was to demonstrate this behavior with ***ChemSep***.

Consider the azeotropic distillation column shown in Figure 1. In one form or another this problem has been studied by many others; indeed, it has become something of a classic. ***ChemSep*** is not able to simulate the column as it should be modeled; with a liquid-liquid decanter following a total condenser for the overhead vapor. The reason is that we have not yet given ***ChemSep*** the ability to handle liquid-liquid phase separation within distillation columns. We can still use ***ChemSep*** to demonstrate multiple steady states for this operation if we omit entirely the condenser and decanter. The reflux from the decanter is modeled as a feed to the topmost stage. There are ***three*** solutions for the set of specifications shown in Figure 1; the students task was to find them.

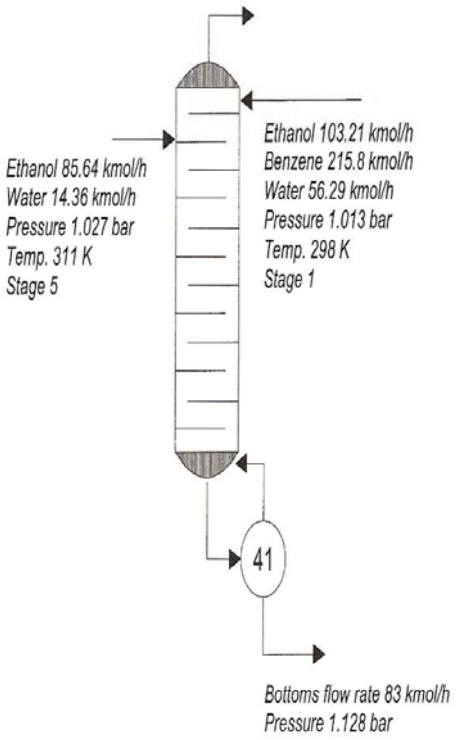


Figure 1. Schematic Diagram of Ethanol - Benzene - Water Column modeled with ChemSep.

These calculations are very sensitive to the choice of VLE model and parameters. Here we will use the DECHEMA / UNIQUAC q' / Antoine combination of models. The UNIQUAC parameters to be entered in the appropriate spreadsheet are as follows:

i	j	A_{ij}	A_{ji}
1	2	-149.57	1131.13
1	3	-163.72	573.61
2	3	2057.42	115.13

ChemSep uses Newton's method to solve all the model equations simultaneously. The initial values of all flows, temperatures and mole fractions are generated by the program with no need for user supplied guess of any quantity at all (although guesses can be provided if needed). Changes to flows, and temperatures from one iteration to another normally are limited to stop the variables from taking on ridiculous values. ***ChemSep*** will not converge this particular problem as posed using the automatically generated initialization combined with the default limits built into the programs algorithm. The problem can be made to converge simply by limiting the allowable changes to flows and compositions between iterations. This is done by pressing *F6* to go to *Solve options*. In that spreadsheet set the default number of iterations to 100 (but don't be alarmed if you sometimes need more than this), the flow limit to 0.3 and the composition step to 0.1. This helps to stop the flows, temperatures and mole fractions from taking on ridiculous values during the computations.

With the input complete we are ready to solve the problem. Press Alt-S to begin the calculations and you should find that ***ChemSep*** converges readily to the solution shown in Figure 2. The students were given the steps needed to obtain this result and asked if this is a good way to operate the column.

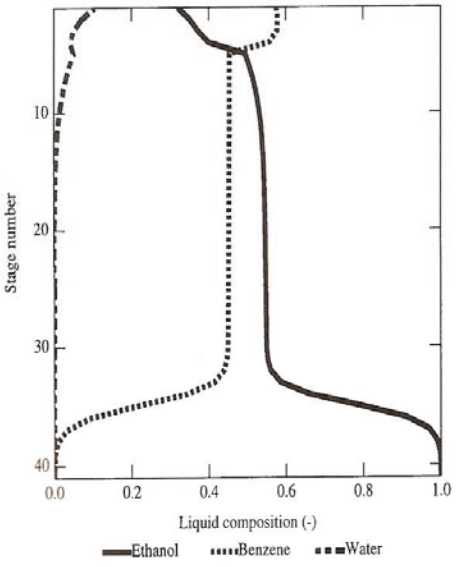


Figure 2. Composition profile corresponding to high purity product.

They were also told how to find a second solution. The steps are as follows:

Set the Murphree efficiency to 0.1 and solve the problem using the *Automatic* initialization.

When the problem has been solved go to *Solve options* and change the initialization option to *Old Results*.

Change the efficiency back to 1 and solve the problem again (just press Alt-S).

The results for this case are shown in Figure 3.

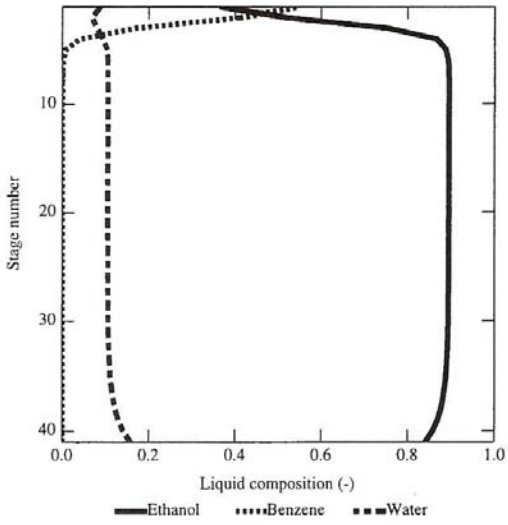


Figure 3. Composition profile corresponding to low purity product.

The students were not told how to find the third solution. In fact, the third solution can be found using an identical method to that used to find the second solution. The only change to the above procedure is to make the default Murphree efficiency equal to 0.83 in step 1 above. The resulting composition profile is shown in Figure 4.

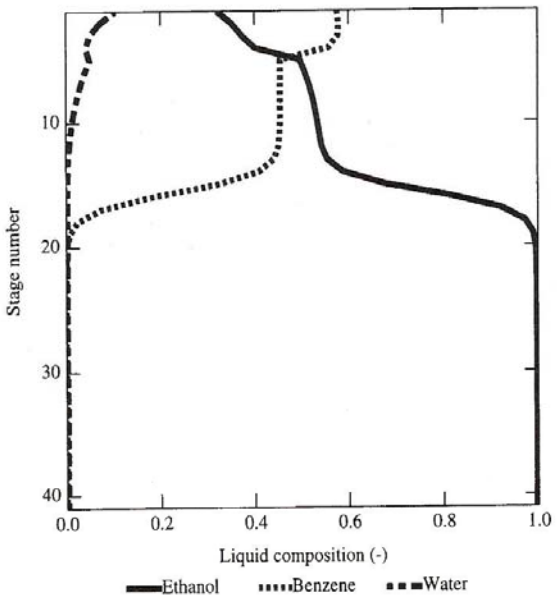


Figure 4. Composition profile corresponding to intermediate purity product.

As part of the exercise the students were asked to think about the consequences for design and operation of a plant that displays this kind of behavior.

Input files for this example (ebw-hi.sep, ebw-lo-sep, and ebw-mid.sep) are available via anonymous ftp from ftp.clarkson.edu in the /pub/chemsep/sepfiles directory.

Further Reading

The problem posed in this article was based on work by, among others,

Magnussen, T., M.L. Michelsen and A. Fredenslund, Distillation 79, 4.2/1 (1979)

Prokopakis, G.J., and W.D. Seider, AIChE J, 29, 49 (1983)

Rovaglio, M. and M.F. Doherty, AIChE J, 36, (1990)

Venkataraman, S., and A. Lucia, Comput. Chem. Eng., 12, 55-69 (1988)

ChemProp

Harry Kooijman, BOC Tech Center
and Ross Taylor, Clarkson University

How can you estimate the density of benzene-toluene liquid mixtures at 2.1 atm?

What is the viscosity of an equimolar acetone-water mixture at 24 Celcius?

How does the thermal conductivity of a butane-pentane gas mixture change with pressure ?

The answer to all of these and many more questions is ***ChemProp***, a program for *estimating* physical and thermodynamic properties. With ***ChemProp*** you may estimate the density, viscosity, thermal conductivity and several other physical properties of pure compounds and mixtures. Methods recommended by Reid, Prausnitz and Poling (Properties of Gases and Liquids, 4th Edition, McGraw-Hill, 1987) as well as by Daubert and Danner (DIPPR Data Prediction Manual, AIChE) and the API data book are included in ***ChemProp***.

ChemProp has been part of the ***ChemSep*** software system available from CACHE since release 3.0 in 1996. The program can be executed from the command line simply by typing cp (or by double clicking on the name cp if you are running Windows). ***ChemProp*** is a DOS program (as is ***ChemSep***) but both of them run quite safely under Windows.

The interface is similar in style to that in ***ChemSep*** so if you are comfortable with that program you will be at home in ***ChemProp***. It uses the same databank of 189 components that comes with ***ChemSep***.

A number of applications of ***ChemProp*** are shown below. It may seem heretical of us to say so but it is possible that ***ChemProp*** is more useful than is ***ChemSep***. Students have used it in sophomore thermodynamics courses, junior separations and fluid mechanics courses, and in senior lab and design courses. We can't even begin to count the hours this program has saved *not* having to answer questions like those on the top of this page.

Example 1

What are the critical properties of methanol?

An extensive list of properties for each pure component are displayed in one window. Nearly 60 constants and temperature dependent properties are displayed for each component. The former includes critical constants, the normal boiling point and many other common properties; the latter includes - but is not limited to - the liquid density, vapour pressure heat of vaporization, liquid and gas heat capacities, viscosities, and thermal conductivities. A very small portion of one such list (for methanol) is shown below.

```
Pure component properties (_ = at 25.00 °C, * =
unknown/can't compute):

Methanol

CH3OH
n-Alcohols Family
Critical temperature (K)                      512.6
Critical pressure (Pa)                     8.09E+06
Critical volume (m3/kmol)                    0.1180
Critical compressibility factor (-)          0.2240
Normal boiling point (K)                      337.9
Melting point (K)                             178.3
Triple point temperature (K)                  175.5
Triple point pressure (Pa)                    0.1115
Molecular weight (kg/kmol)                    32.04
Liquid molar volume at normal boiling
point (m3/kmol)                            0.04070
Acentric factor (-)                          0.5589
Radius of gyration (m)                     1.53E-10
Solubility parameter (_(J/m3))             2.95E+04
Dipole moment (Coulomb.m)                  5.67E-30
Van der Waals volume (m3/kmol)              0.02171
Van der Waals area (m2/kmol)               3.58E+08
IG heat of formation (J/kmol)              -2.0E+08
IG Gibbs energy of formation (J/kmol)      -1.6E+08
```

The units, format and number of significant digits displayed can be set by the user.

Example 2

What are the properties of an equimolar mixture of methanol, chloroform, methylacetate?

Mixture properties may also be estimated by ***ChemProp***. The composition, temperature and pressure must be specified and property models selected (or the program will make its own - usually sensible - choices if you don't). The results are summarized in another window as illustrated below. Also reported (but not shown here) is a summary of the methods used to estimate the mixture properties.

Component fractions:	Mole	Mass
Methanol	0.3333	0.1421
Chloroform	0.3333	0.5294
Methylacetate	0.3333	0.3285
Temperature 25.00 (°C)		
Pressure 1.013 (bar)		
Mixture properties:	Liquid	Vapour
Molar mass (kg/kmol)	75.17	75.17
Molar density (kmol/m3)	15.23	0.04254
Density (kg/m3)	1145	3.197
Viscosity (N.s/m²)	4.75E-04	1.01E-05
Heat capacity (J/K/kmol)	1.12E+05	6.54E+04
Thermal conductivity (J/m/K/s)	0.1569	0.01139
Surface tension (N/m)	0.02448	

Example 3

What is the vapor pressure of methanol, chloroform, and methylacetate at 25 and 125 Celcius?

Temperature dependent properties can also be tabulated and plotted and both forms can be displayed and printed. Below we show part of a table that reports the vapor pressure of each component in our example mixture. The actual table included values computed for temperatures 2 degrees apart from 25 to 125 Celcius - the range and number of points is, of course, up to the user to modify as needed.

Temperature (°C)	Methanol Vapour pressure (bar)	Chloroform Vapour pressure (bar)	Methylacetat Vapour pressure (bar)
25.00	0.1684	0.2616	0.2857
35.00	0.2790	0.3958	0.4380
45.00	0.4456	0.5801	0.6505
55.00	0.6889	0.8266	0.9389
65.00	1.034	1.149	1.321
75.00	1.512	1.562	1.817
85.00	2.157	2.081	2.448
95.00	3.013	2.723	3.237
105.0	4.125	3.507	4.208
115.0	5.547	4.452	5.388
125.0	7.340	5.579	6.804

The new version to be included with the next release of ***ChemSep*** (in May 1997) includes some significant additions including thermodynamic properties (activity coefficients, for example, as shown in Figure 1), and the ability to compute and display bubble and dew point diagrams for binary (Figure 2) and ternary mixtures (Figure 3).

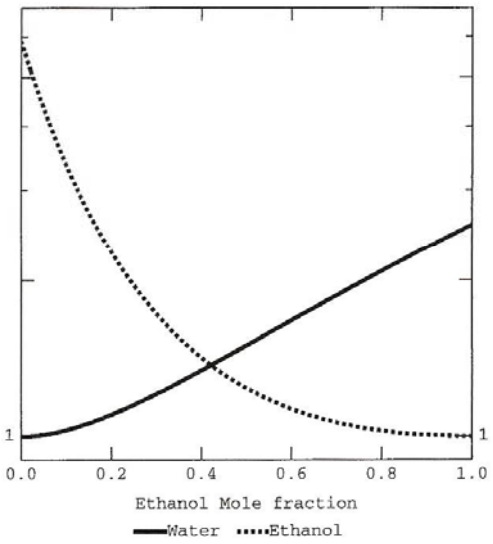


Figure 1. Activity coefficients for ethanol - water mixture computed using the Van Laar model.

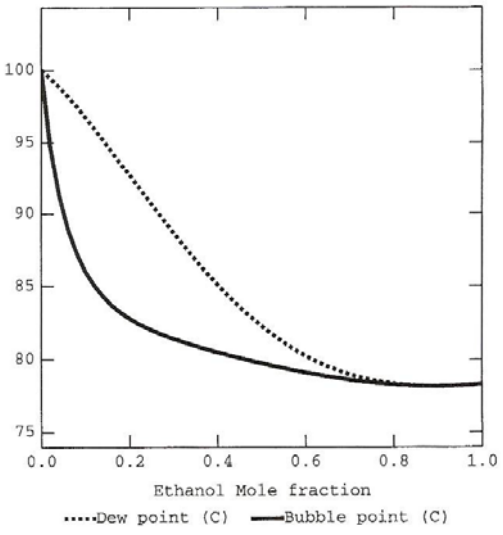


Figure 2. Txy diagram for ethanol - water mixture computed using the Van Laar model.

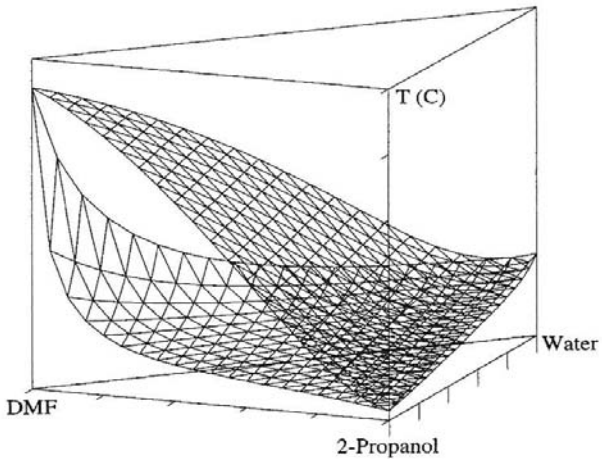


Figure 3. Txy surface for a mixture of 1-propanol - water - DMF computed using the Wilson model.

ChemLib

The library of components that comes with the CACHE version of ***ChemSep*** contains data for 189 different components. For some of you this is simply not enough and you have asked if it is possible to add components to the databank.

Until the next release of ***ChemSep*** the answer is no. However, the next release will include ***ChemLib***, our physical property library management program. As is the case with both of the other two components of the ***ChemSep*** system, it is a DOS program (but runs safely under Windows). ***ChemLib*** allows users easy inspection (and alteration) of the property constants and temperature dependent property correlation parameters used in ***ChemSep*** and ***ChemProp***. The program can also be used to add (remove) components to (from) a databank. Property data can be exported and imported in a variety of formats including plain text and the binary file format used in our own databank. Thus, the program can be used to create entirely new databanks with as many additional components as desired.

Picles + Digest = Control Station™ for Windows

Doug Cooper† *and Manish Sinha*
University of Connecticut

Picles and Digest, the popular software packages now used in over 100 colleges and universities around the world for control system design, analysis and training, has just been made better. The reason is that these two packages have been combined into a single, integrated environment which retains all of the features of Picles and Digest while providing a host of exciting new capabilities. We are pleased to introduce the new Control Station™ for Windows!

Control Station is a point-and-click environment developed to be compatible with Windows 3.1, Windows 95 and Windows NT as well as the popular computer networks. The main screen, shown in Figure 1, reveals that Control Station is comprised of three modules: *Case Studies*, *Design Tools* and *Customize Process*.

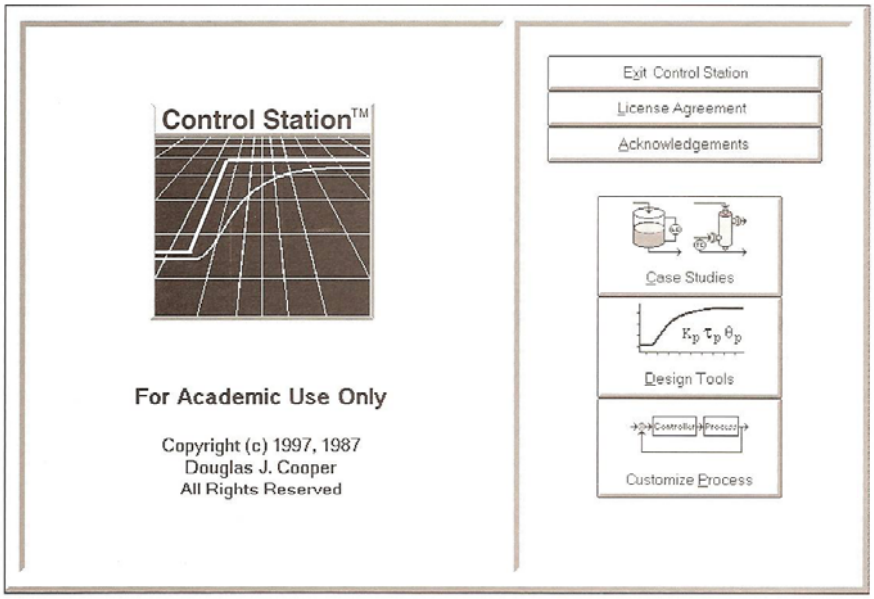
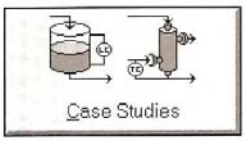


Figure 1. Control Station's main screen.

† Author to whom correspondence should be addressed

Case Studies Module

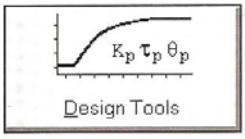


The pedagogical approach behind the *Case Studies* module is that hands-on experience is crucial to learning the abstract and mathematical subject of automatic process control. *Case Studies* offers easy-to-use and visually appealing simulations which can be used to study a wide range of process dynamics and control concepts. The processes available in *Case Studies* include Gravity Drained Tanks, Pumped Tank, Heat Exchanger, Jacketed Stirred Reactor, and Distillation Column.

Each of these simulations is animated in color-graphic display to provide you with extensive and inexpensive "real world" experiences. You can manipulate process variables in open loop to obtain pulse, step, sinusoidal or ramped test data. Process data can be recorded as printer plots or disk files for process modeling and controller design studies. The *Design Tools* module discussed later is well suited for this modeling and design task.

The controllers available enable the exploration and study of increasingly challenging concepts in an orderly fashion. Early concepts include studying basic dynamic behaviors such as process gain, time constant and dead time. Intermediate concepts include the tuning and performance capabilities of the range PID controllers. Advanced concepts include cascade, feed forward, decoupling, digital and model predictive control.

Design Tools Module



The *Design Tools* module offers several tools for controller design and analysis. One important feature is the ability to regress dynamic models to tables of process data. *Design Tools* can import such data from Control Station's *Case Studies* and *Customize Process* simulations as well as from other software packages and real processes. To do so, the data must be in text file (ASCII) form with data columns separated by tabs, commas or spaces

With just a few clicks, you mark which data column contains the manipulated variable data, which contains the measured process variable data, and which contains the time stamp data. The linear models available in the *Design Tools* model library include:

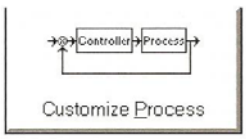
First Order Plus Dead Time
First Order Plus Dead Time with Integrator
Second Order Overdamped Plus Dead Time
Second Order Overdamped Plus Dead Time and Lead Time
Second Order Underdamped Plus Dead Time

The process data is modeled by minimizing the sum of squared errors (SSE) between the actual measured response and the predicted model response when using the actual manipulated variable process data contained in the file. In computing the SSE, *Design Tools* assumes that the process is at steady state before the dynamic event occurs and that the first data point in the file is a good median value of that initial steady state.

A second important capability in *Design Tools* is the computation of P-Only, PI and PID controller tuning values based on dynamic model parameters. The library of popular tuning correlations include Cohen-Coon, internal model control (IMC), integral of absolute error (IAE) and integral of time-weighted absolute error (ITAE).

In modern control installations, the dynamic models regressed by *Design Tools* can be used directly in advanced controllers ranging from a simple Smith predictor up through the full model predictive control (MPC) algorithms. *Design Tools* can also be used to design feed forward elements. For feed forward designs, it is the disturbance variable which should be stepped, pulsed or otherwise perturbed. This disturbance data then becomes the manipulated variable when regressing the disturbance-to-measured variable dynamic model.

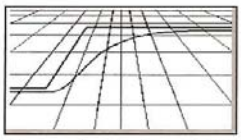
Customize Process Module



The *Customize Process* module is a block oriented environment that enables you to implement a process and controller architecture to your own specifications for a wide range of custom control investigations. The simulations can be for single loop processes using a transfer function for the process and another for the load disturbance. Such single loop architectures permit a host of PID, feed forward, digital control and model predictive control studies. You can investigate the benefits and drawbacks of different controller modes and different tuning parameter values in "what if" scenarios, or maybe study the sensitivity of your design to plant/model mismatch, or perhaps isolate and explore the impact of noise in the measured variable on closed loop performance.

The Customize Process module also lets you assemble multiple transfer function and controller blocks to study cascade, ratio, and multivariable systems. Here, a library of controller diagrams are available for your convenience. All you have to do is enter the transfer function values for your particular application. The transfer functions for both single and multiple loop architectures are entered into Control Station with user friendly dialog boxes. *Design Tools* is perfect for regressing transfer functions to process data from your plant or lab.

A Brief Tour



The heat exchanger process, shown in Figure 2, is one of the case studies in Control Station. The heat exchanger simulates a counter-current lube oil cooler. The manipulated variable is the flow rate of cooling water on the shell side. the measured process variable is lube oil temperature exiting the exchanger on the tube side. This process has a negative process gain and exhibits a nonlinear behavior as operating level changes. Also, changes in the flow rate of the warm oil disturbance stream, which mixes at the entry to the exchanger, cause an inverse or nonminimum phase open loop response in the measured process variable.

Figure 2 shows a snapshot of the screen, including a process graphic and two strip charts. The lower strip chart displays a series of pulses in the controller output signal. These pulses were made to generate the data required for the subsequent dynamic modeling and controller tuning steps. The top strip chart displays the measured exit temperature as it responds to the changes in the controller output signal. As indicated at the bottom right of Figure 2, the data is being collected in a disk file called DEMO.DAT.

Both strip charts scroll across the screen and the process graphic data boxes continually update to create the illusion of a control room setting as you explore and learn. The changes to controller output were made in Figure 2 by clicking on the cooling flow rate box on the process graphic and entering the different values.

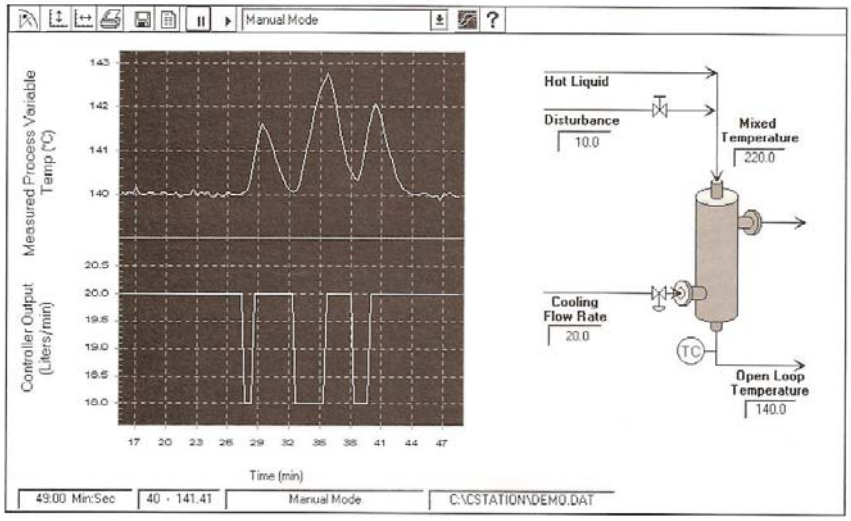


Figure 2. Case Studies' Heat Exchanger generates dynamic data in manual mode.

The next step in the classical controller design procedure is to regress a dynamic model to the process data. With just a few clicks, the DEMO.DAT data file is processed by *Design Tools*, a first order plus dead time (FOPDT) model is selected from the library of models, and a regression is performed. The result is shown in Figure 3.

In just a few more clicks, *Design Tools* uses the FOPDT model parameters in its library of popular controller tuning correlations to yield P-Only, PI and PID tuning recommendations. The list of tuning values for a PI controller are shown in Figure 4.

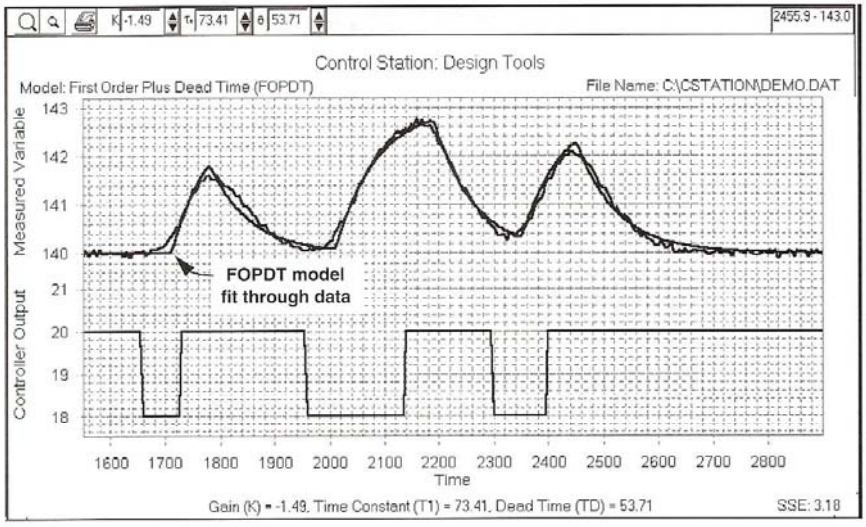


Figure 3. Design Tools regresses a FOPDT dynamic to Heat Exchanger data.

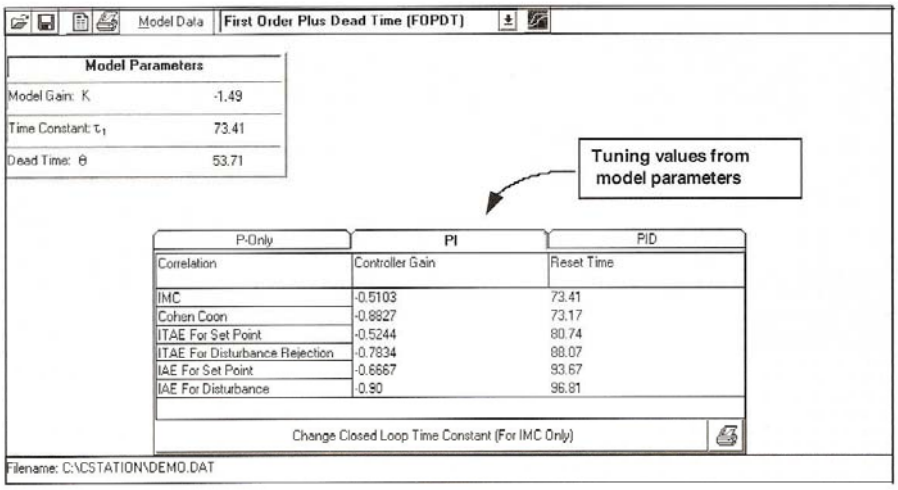


Figure 4. Design Tools computes controller tuning values based FOPDT model parameters.

To implement the controller, return to Control Station's heat exchanger case study and double click on the temperature controller symbol (the "TC" with the circle around it shown on the process graphic). As shown in Figure 5, a controller tuning menu pops up for convenient selection of the control law and input of the tuning parameters. Finally, the set point tracking performance of the controller is tested by clicking on the set point box on the process graphic and entering desired values for this parameter. The result of this performance test is shown in Figure 6.

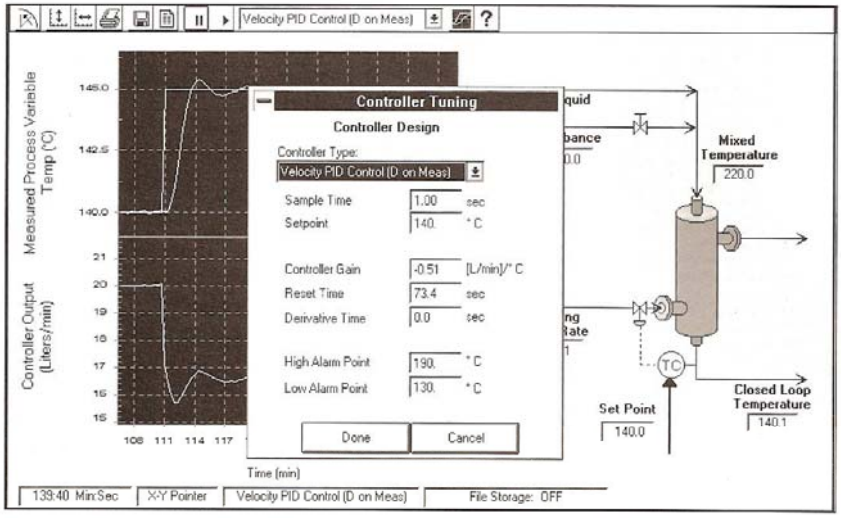


Figure 5. PI controller is implemented using a pop up menu.

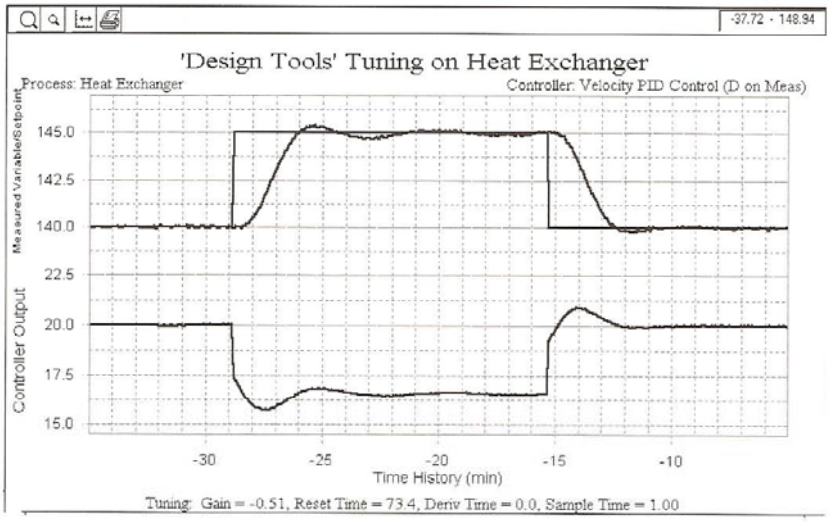


Figure 6. Performance of PI controller tuned using Design Tools.

Available This Summer

Control Station is scheduled for release on August 1, 1997. When used for teaching college students, a department site license for CACHE members is $125 the first year and $95 per year in subsequent years. For nonmembers, Control Station is $125 per year. An academic department site license entitles students and faculty within a department to make unlimited copies of the program for educational use.

For more information about Control Station, its features and capabilities, and its use in education and training, please contact:

Doug Cooper
Chemical Engineering Department
University of Connecticut, U-222
Storrs, CT 06269-3222
Phone: (860) 486-4092
E-mail: cooper@eng2.uconn.edu

ANNOUNCEMENTS

1997 American Control Conference
June 4 - 6, 1997
Albuquerque, New Mexico

The 1997 American Control Conference will be held in Albuquerque, New Mexico at the Albuquerque Convention Center, The Hyatt Regency Hotel and The Albuquerque Doubletree Hotel. The conference will have 915 refereed papers and 8 technical workshops representing a strong interest in the field of control engineering. The technical program will feature industrial and applications presentations from the aerospace, process control, robotics, automotive, manufacturing and metals communities. There will also be development and theory presentations from areas such as fault detection, estimation, and robust, and predictive control.

Plenary speakers and topics are:

Professor Graham C. Goodwin, Dean of the Faculty of Engineering, and Director of the Center for Integrated Dynamics and Control at the University of Newcastle, Australia
"Defining the Performance Envelope in Industrial Control".

Dr. Andrew Packard, Associate Professor in Mechanical Engineering at the University of California, Berkeley
"Theory and Design Experiences with Linear Parameter Varying (LPV) Control".

Professor Rolf Iserman of the Institute of Automatic Control, Darmstadt University of Technology, Germany
"Mechatronic Systems - A Challenge for Control Engineering"

The workshops also range from practice (fault detection, automotive) to developments (fuzzy control, neural networks) to techniques (robust control, large scale systems, and unified linear control formulation).

There are a number of enjoyable social events which feature New Mexican food and culture, Albuquerque, on the Rio Grande River and near to the Sandia Mountains, offers historic missions, art galleries, southwest charm, a diverse heritage, and tasty New Mexico cuisine. Trips to neighboring Santa Fe will be uniquely remembered by participants and their families.

For details and registration forms view our homepage at http://www.eece.unm.edu/controls/ACC97/welcome.html or send an e-mail inquiry to:
rhinehart@coel.coe.ttu.edu or contact:

General Chair
Naim A. Kheir - ACC97
Oakland University
Dept. of Electrical & System Engr.
Rochester, MI 483098-4401
(810) 370-2177 or FAX (810) 370-4633
kheir@vela.acs.oakland.edu

Registration Chair
M. Edwin Sawan
Wichita State University
Dept. of Electrical Engineering
Wichita, KS 67260—0044
(316) 978-3415 or FAX (316) 978-3853
ed@shocker.ee.twsu.edu

Workshop Chair
Michael K. Masten -ACC97
Texas Instruments
2309 Northcrest
Plano, TX 75075
(214) 995-7986 or FAX (214) 995-2770
m.masten@ieee.org

Industrial Contributors to CACHE

The following companies have recently contributed financial support to specific CACHE activities.

3M
Aspen Technologies
Dupont
Hyprotech
Merck & Co.
Simulation Sciences

ANNOUNCEMENTS

First Announcement

FOCAPO 98

July 5 - 10, 1998 Snowbird, Utah

About the Conference

The Foundations of Computer Aided Process Operations Conferences (FOCAPO 98) to be held in Snowbird, Utah from July 5-10, 1998 will be the third in a series of conferences dealing with the use of computers in support of process operations. Since the first FOCAPO conference in Park City, Utah in 1987 and the second in Crested Butte, Colorado in 1993 and given the developments in the process industry and computer technology there has been an enormous increase in interest in improving the efficiency and effectiveness of process operations. In fact, without much danger of exaggeration, one can assert that much of the restructuring within the process industry over the past few years has been operations focused. Given the likely continuation of this trend and the host of related research and technical issues, FOCAPO 98 will bring together practitioners, management, and researchers for a comprehensive look at the state of the art in computer aided process operations, a discussion of strategies important to thriving in an environment of continuous change and rapidly advancing technology, and the important challenges to be overcome.

The goals of FOCAPO are to:

1) provide a forum for practitioners, management, and researchers to share their experience

2) emphasize presentations describing technology that is being reduced to practice or is likely to be in the next five years

3) provide an opportunity for industrial practitioners, academics, and vendors to interact

4) motivate future research by describing problems that are intractable or expensive to solve with existing approaches and by describing new application areas.

The program will reflect an international perspective to correspond to the globalization of the process industry.

Conference Topics

The conference is organized into problem oriented sessions with the following titles:

1) Plant Wide Optimization
2) Pilot Plant Operations
3) Emerging and High Growth Processes (e.g. biological, electronic fabrication, etc.)
4) Technological Challenges to Next Generation Supply Chain Management
5) Planning/Scheduling of Multiproduct Plants
6) Environmental Issues
7) Next Generation Enabling Technology: Trends and Deployment Issues
8) Product Integrity/Quality

Technology Issues

Discussion of core enabling technologies in the context of key operations problems will be an important part of FOCAPO 98. In particular, the sessions will encompass the following enabling technologies:

1) optimization methods
2) planning/scheduling
3) process control as a tool for achieving high level operations objectives
4) knowledge based systems/neural networks
5) simulation software
6) information technology
7) probability and statistics
8) computer interfaces/software issues
9) on-line instrumentation/process monitoring
10) abnormal/exceptional situation management
11) risk analysis
12) accomodating data uncertainty.

Although the focus of each session will be problem and issue oriented rather than focusing on technology alone, FOCAPO 98 will continue the tradition of past such conferences by informing participants about technology trends and challenges that will have an important impact on process operations in the near future.

Conference participants are encouraged to submit papers addressing topics and/or technical issues to the contributed paper session.

ANNOUNCEMENTS

Session Format

Each of the sessions will be patterned around the following format to provide both an informative overview of topics as well as a significant opportunity for broad based audience participation.

- A presentation defining the area, including a description of the current state of the relevant enabling technologies and potential future development.
- A presentation of what is being practiced in operations today (with examples) and the opportunities for future applications.
- A panel consisting of the speakers and several other conference participants will convene for the remaining time allocated to the session. Non- speaker panel members will have an opportunity to comment on the earlier presentations. Afterwards, questions from the audience will be directed to the speakers or other panel members.

Contributed Papers Session

In addition to the speaking oriented sessions, one afternoon of the conference will be devoted to a fair involving thirty to forty contributed papers from conference participants.

Call for Abstracts for Contributed Papers

If you would like to participate in the contributed paper session, please send a 500-word abstract by postal mail or e-mail to the session chair by December 1, 1997.

Chair:
Professor Ignacio Grossmann
Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
e-mail: grossmann@cmu.edu

Vendor Demonstrations

During the afternoon periods of the conference and while formal programming is not in session, conference participants will have the option of visiting vendor booths for product demonstrations and discussions about commerical technology.

Conference Organizers

Gary Blau
DowElanco
9330 Zionsville Rd
Indianapolis, IN 46268
gblau@dowelanco.com

Joseph Pekny
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907-1283
pekny@ecn.purdue.edu

Technical Planning Committee

Kun Soo Chang	Pohang University (Korea)
James Downs	Eastman Chemical (USA)
Ignacio Grossmann	Carnegie-Mellon (USA)
Iori Hashimoto	Kyoto University (Japan)
Simon Jones	BASF (Germany)
Hank Kohlbrand	Dow Chemical (USA)
Lowell Koppel	Aspen Technology (USA)
Mark Kramer	Gensym Corp (USA)
Philip Law	ETH (Switzerland)
Kristian Lien	Norwegian Univ. (Norway)
Wolfgang Marquardt	Aachen Technical (Germany)
Bernard McGarvey	Eli Lilly & Co (USA)
Gregory McRae	MIT (USA)
Manfred Morari	ETH (Switzerland)
John Perkins	Imperial College (UK)
Malcolm Preston	ICI PLC (UK)
Luis Puigjaner	U. Politec Catalunya (Spain)
David Smith	DuPont (USA)
Moe Sood	Mobil (USA)
George Stephanopoulos	MIT (USA)
Jeff Siirola	Eastman Chemical (USA)
(CACHE Corporation Representative)	
Scott Keeler	DowElanco (USA)
(CAST/AICHE Representative)	

ANNOUNCEMENTS

Location

Just a forty minute drive from the Salt Lake International airport, Snowbird is located in the Cottonwood Canyon in the heart of the Wasatch Mountain Range. Shuttle service is easily arranged from the airport to this beautiful resort area. Snowbird is also just a thirty minute drive from Salt Lake City.

Since everything is within walking distance, you may not need a car. The Snowbird village offers many facilities from restaurants to shopping. If you are looking for recreational activities, Snowbird offers many outdoor and indoor activities from swimming, golf, tennis, and racquet ball. There is also a health spa which offers everything from body massages to facials and herbal wraps.

If being outdoors with nature is more of what you want, take a naturehike or go mountain biking on the many trails along the mountainside. There is also an aerial tram ride where you can enjoy the beautiful view up to Hidden Peak.

The 57,000 square foot conference area located in the Snowbird Resort will create a tranquil environment. Technical sessions will be held in the mornings and evenings, leaving the afternoons free.

Hotel fees will range from $90 to $144 per night. Actual rates will be available upon registration.

Inquiries

For more conference information please direct e-mail to the following address:

focapo98@ecn.purdue.edu

Or visit the FOCAPO98 web site for updated information:

http://che.www.ecn.purdue.edu/FOCAPO98/

Preregistration for FOCAPO 98

Preregistration is required to attend FOCAPO98. The conference fee of $675 will include registration, proceedings, opening reception, conference banquet, and daily refreshments. Do not send fees at this time.

Please complete and return this preregistration form, no later than January 2, 1998 to:

Attn: Janet Taylor
CHME 112
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907-1283

Name: _____
Title: _____
Affiliation: _____
Mailing Address:
_____
_____
_____
_____
Telephone: _____
E-mail: _____
Fax: _____
Research Interests:
_____
_____
_____
Reasons for wishing to attend conference:
_____
_____
_____
_____
_____
_____
_____

ANNOUNCEMENTS

New CACHE Trustee

Peter T. Cummings

Peter T. Cummings received his B. Math. (with First Class Honors and University Medal) from the University of Newcastle (Australia) in 1976, and his Ph.D. in applied mathematics from the University of Melbourne (Australia) in 1980. After post-doctoral appointments in Physics at the University of Guelph (Ontario, Canada) in 1980 and in Chemistry and Mechanical Engineering at the State University of New York at Stony Brook, 1981-83, he joined the Department of Chemical Engineering at the University of Virginia as an Assistant Professor in 1983, attaining the rank of full professor in 1991. In January, 1994, he assumed his current joint position as Distinguished Professor in the Department of Chemical Engineering at the University of Tennessee and Distinguished Scientist in the Chemical Technology Division at Oak Ridge National Laboratory. Professor Cummings is the recipient of many awards, including a prestigious Commonwealth Scientific and Industrial Research Organization Post-Doctoral Fellowship from the Australian government in 1980, a Camille and Henry Dreyfus Foundation Research Award for Newly Appointed Faculty in the Chemical Sciences in 1983, the inaugural Gold Medal for Professional Excellence awarded by the Convocation (alumni association) of the University of Newcastle in 1988, and co-recipient of the University of Virginia President's and Board of Visitors' Prize for outstanding research in the life sciences in 1996. Since 1991, he has been a member of the editorial boards of two international statistical mechanics journals, Molecular Physics and Fluid Phase Equilibria. He is a member of the American Physical Society, American Institute of Chemical Engineers, American Chemical Society, Sigma Xi, Society of Rheology, and Materials Research Society. He has held several visiting positions: Visiting Fellow in the Research School of Chemistry at the Australian National University in Canberra, Australia, Distinguished Visiting Scholar in the Department of Chemical Engineering at the University of Massachusetts, and Faculty Research Participant in the Oak Ridge Associated Universities Program at Oak Ridge National Laboratory.

Professor Cummings is well-known for his research on molecular approaches to predicting physical properties in systems of industrial interest, such as supercritical aqueous solutions, alkane fluids, and polymer solutions. He is among the leaders in the application of massively parallel supercomputers to predicting thermophysical properties. In recent years, in collaboration with Roseanne Ford of the University of Virginia, he has been applying concepts from the statistical mechanics of transport processes to the description of bacterial migration in porous media. Professor Cummings is the author of over 150 refereed publications, a frequent invited speaker at international conferences and a consultant to several companies. His research is supported by the National Science Foundation (Chemical and Thermal Systems Division and Engineering Education and Centers Division), the Department of Energy Chemical Sciences Division, the Department of Energy Environmental Management Science Program, Lockheed-Martin Energy Research Corporation and the Chemical Technology Division and the Chemistry and Analytical Sciences Division of Oak Ridge National Laboratory. He has been a past recipient of grants from the Dreyfus Foundation, the Petroleum Research Fund, the Virginia Center for Innovative Technology, Aqualon Company (a joint venture of Hercules and Henkel), Exxon Educational Foundation, Linnhoff-March Consulting, and Commonwealth Aluminum Company (COMALCO) of Australia.

Catalog of Products

To order CACHE products, complete the standard order form and send with payment to:

CACHE Corporation
P.O. Box 7939
Austin, TX 78713-7939

FAX: (512) 295-4498

We now take Credit Card Orders
Visa/Mastercard only

If you would like to receive a current CACHE Products Catalog, send a message to <cache@uts.cc.utexas.edu>, call (512) 471-4933, or write to the address listed above.

STANDARD ORDER FORM

CACHE Product Description	Qty.	Supporting	Non-Supporting	Total
AI Monograph - Volumes 1, 2, 3 & 4 (sold separately)		$20	$25	
AI Monograph Set (Volumes 1-4)		$50	$75	
AI Case Study - Volumes 1, 2, & 3 (sold separately)		$10	$17	
AI Case Study Set (Volumes 1-3)		$20	$35	
CACHE Tools - Model Predictive Control Toolbox Manual and 3.5" PC disk		$160	$250	
CD-ROM - Volume 1 (CACHE 25th Anniversary) Student chapters and supporting departments Individual students and faculty Individuals with no academic connection		$5	 $10 $35	
CD-ROM - Volume 2 Student chapters and supporting departments Individual students and faculty Individuals with no academic connection		$15	 $20 $50	
ChemSep Version 3.1 • without documentation • with documentation **(License agreement must be signed first)**		 $100 + annual $60 $135 + annual $60	 $115 + annual $75 $150 + annual $75	
GPSS **(License agreement must be signed first)**		$25	$25	
Interactive Computer Modules • per course • set of four		 $35 $100	 $75 $200	
MultiBatchDS Two (2) 3.5" PC disks Manual **(License agreement must be signed first)**		 $90 + annual $50 $10	 $120 + annual $75 $10	
Picles Version 3.1 **(License agreement must be signed first)**		$95 + annual $75	$115 + annual $95	
PIP		$50	$75	
Polymath Version 4.0		$125 + annual $75	$150 + annual $100	
Process Design Case Study - Volume 1 Process Design Case Study - Volume 2 Process Design Case Study - Volume 3 Process Design Case Study - Volume 4 Process Design Case Study - Volume 5 Process Design Case Study - Volume 6 (with GAMS users guide)		$15 $15 $15 $15 $20 $55	$35 $35 $35 $35 $40 $80	
Purdue Laboratory Simulation Software Modules (Dow, Amoco, Eastman, Mobil)		$225 per module plus annual $25	$225 per module plus annual $25	
Strategies for Creative Problem Solving • personal use only • domestic universities • overseas universities • industrial companies Problem Solving Slides (pc or mac) • domestic • overseas		 $65 $90 $90 $15 $19	 $65 $90 $105 $210/machine $15 $19	
Target II **(License agreeement must be signed first)**		$5	$5	
THEN		$5	$5	
			TOTAL	

Prepayment is required
Overseas orders are sent surface at no charge. Airmail is extra.

Name: _____
Address: _____
_____
E-Mail : _____
Phone: _____

<u>Payment</u> (please check)

__ check (US funds, US bank)
__ Purchase Order
__ Credit Card
Card No: _____
Exp Date: _____
Exact Name on Card: _____

Make checks payable to:
CACHE Corporation
P.O. Box 7939
Austin, TX 78713-7939

Signature: _____

E-Mail: cache@uts.cc.utexas.edu **Fax:** (512) 295-4498 **Phone:** (512) 295-2708 or (512) 471-4933

Chemical Engineering Departments Supporting CACHE

CACHE annually solicites universities for funds to carry out on-going CACHE activities and nurture new projects. The following is a list of our generous supporters

University of Alberta
University of Arizona
University of Arkansas
University of Akron
University of Bahrain
University of Bath
University of British Columbia
University of Calgary
University of California, Davis
University of California, Irvine
University of California, Santa Barbara
University of Cambridge
University of Cape Town
University of Cincinnati
University of Colorado
University of Connecticut
University of Dayton
University of Delaware
University of Houston
University of Idaho
University of Illinois, Chicago
University of Illinois, Urbana
University of Iowa
University of Kansas
University of Kentucky
University of Laval
University of Louisville Speed Scientific School
University of Maine
University of Manchester Institute of Science & Technology
University of Maribor
University of Maryland
University of Massachusetts, Amherst
University of Massachusetts, Lowell
University of Michigan
University of Minnesota
University of Minnesota, Duluth
University of Mississippi
University of Missouri, Columbia
University of Missouri, Rolla
University of Nebraska
University of Nevada, Reno
University of New Brunswick
University of Newcastle
University of New Hampshire
University of New Haven
University of New Mexico
University of New South Wales
University of North Dakota
University of Notre Dame
University of Oklahoma
University of Ottawa
University of Oulu
University of Pennsylvania
University of Pittsburgh
University of Queensland
University of Rhode Island
University of Saskatchewan
University of Sherbrooke
University of South Alabama
University of South Carolina
University of South Florida
University of Southern California
University of Southwestern Louisiana
University of Sydney
University of Teesside
University of Texas at Austin
University of Toledo
University of Toronto
University of Tulsa
University of Utah
University of Virginia
University of Washington
University of Waterloo
University of Wisconsin
Vanderbilt University
Villanova University
Virginia Polytechnic Institute
West Virginia Institute of Technology
Washington State University
Washington University
Wayne State University
West Virginia Graduate College
West Virginia University
Widener University
Worcester Polytechnic Institute
Yale University
Yonsei University

Chemical Engineering Departments Supporting CACHE

CACHE annually solicites universities for funds to carry out on-going CACHE activities and nurture new projects. The following is a list of our generous supporters

Arizona State University
Brandenburg Tech. Univ. of Cottbus
Brigham Young University
Bucknell University
California Institute of Technology
California State Polytechnic University, Pomona
Carnegie-Mellon University
Case Western Reserve University
Christian Brothers University
Chulalongkorn University
City College of New York
Clarkson University
Clemson University
Cleveland State University
Colorado School of Mines
Colorado State University
Cork Regional Technical College
Cornell University
Curtin University of Technology
Danmarks Tekniske Universitet
Dartmouth College
Drexel University
Dublin City University
Ecole Polytechnic-University of Montreal
Eidgenossiche Technische Hochschule (ETH)
Eindhoven University of Technology
Florida Institute of Technology
Georgia Institute of Technology
Groningen University
Hampton University
Helsinki University of Technology
Hong Kong University of Science & Tech.
Illinois Institute of Technology
Indian Institute of Technology
Instituto Tecnologico de Celaya
Iowa State University of Science & Tech.
Johns Hopkins University
KAIST
Kansas State University
Kasetsart University
King Abdulaziz University
King Mongkut's Inst. of Tech. Thonburi
Lafayette College
Lakehead University
Lamar University
Lappeeranta University of Technology
Lehigh University
Loughborough University of Technology
Louisiana State University
Louisiana Tech University
Manhattan College
Massachusetts Institute of Technology
McGill University
McMaster University
McNeese State University
Michigan State University
Michigan Technological University
Middle East Technical University, Turkey
Mississippi State University
Monash University
National Cheng Kung University
National Taiwan Institute of Technology
New Jersey Institute of Technology
New Mexico State University
North Carolina Agricultural & Technical State University
North Carolina State University of Raleigh
Northeastern University
Norwegian Institute of Technology
Ohio State University
Ohio University
Oklahoma State University
Oregon State University
Pennsylvania State University
Polytechnic University
Princeton University
Purdue University
Queen's University
Rensselaer Polytechnic Institute
Rice University
Rose-Hulman Institute of Technology
Rowan College
Royal Melbourne Institute of Technology
Royal Military College of Canada
Rutgers State University
San Jose State University
South Dakota School of Mines & Technology
Stevens Institute of Technology
Swiss Federal Institute of Technology (EPFL)
Syracuse University
Technion-Israel Institute of Technology
Texas A&M University
Texas Tech. University
Thermische Verfahrenstechnik der Tech.
Tri-State University
Tufts University
Tuskegee University
Universidad de Concepcion
Universidad Michoacana
Universidad do Minho
Universidad Nacional de la Plata
Universidad Nacional de Mar del Plata
Universität Erlangen-Nürnberg
Universitat GH - Essen
Universitat Kaiserslautern
Université de Sherbrooke
University College London
University of Adelaide

Topics in this issue of the CACHE Newsletter:

CACHE Corporation
P. O. Box 7939
Austin, TX 78713-7939

Nonprofit Organization
U.S. Postage Paid
Austin, TX
Permit No. 699