CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 45 FALL 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:

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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.

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CACHE NEWS

No. 45 Fall 1997

Important Notice

As an experiment, this issue of CACHE News contains only highlights of CACHE activities during the last six months. Detailed information can be found on the CACHE web site: http://www.che.utexas.edu/cache.

Please let us know of any comments or suggestions about this experiment via e-mail to: cache@uts.cc.utexas.edu

Visual Basic for Applications, Add-Ins and Excel 7.0

Edward M. Rosen
EMR Technology Group

The availability of Visual Basic for Applications (VBA) as its macro language gave to Excel 7.0 (the version in Microsoft Office 95) a powerful computational capability. The macro language, originally designed as a method of recording keystrokes, enables the user to write computationally significant routines that can be made an integral part of the spreadsheet.

The VBA language (1, 2) has been described as both a subset and superset of Visual Basic. It was first made available for Excel 5.0 (3) but has been extended as the macro language for all of MicroSoft's Office products in Office 97.

Despite the popularity of the spreadsheet as a computational tool in academia (4, 5, 6, 7) little use appears to have been made of the VBA language either to simplify the coding of the spreadsheet or to enhance the spreadsheet's capabilities.

Worksheet and Array Functions

Excel has a large number of *built-in worksheet functions.* These functions are of two kinds.

The first are those which return a single value. These functions are evoked directly by selecting a cell and then placing an "=" sign followed by the name of the function and any arguments which are required. The **Enter** key is then pushed. Included are such routines as COS, EXP and MIN.

The second type of built-in worksheet function is those which return an array of values. These are called *array functions* and are evoked by first selecting the array of cells into which the output of the function will be placed. Then an "=" sign is placed in the first cell (or in the formula bar) followed by the name of the function and any arguments. Rather than pushing the **Enter** key the **Shift+Ctrl+Enter** key is entered. Included in this type of function are MINVERSE and LINEST.

Add-Ins

Add-Ins are files that can be installed to add commands and functions to Excel.

The *Analysis Toolpak is* a large collection of special worksheet functions that are used just like the built-in functions. However, it must be specifically included by checking it in the Tools → Add-Ins dialog box.

Included in A*nalysis Toolpak* are such functions as ERF and BESSELK.

The *Analysis ToolPak - VBA* is a similar collection of functions that can be called from the VBA language. They are indicated in partial lower case form with names such as Erf and Besselk. To make these functions available, the location of the file ATPVBAEN.XLA must be specified by placing a check opposite the file in the Tools → References dialog box.

Both built-in and add-in functions can be viewed by clicking on the **Function Wizard.** They appear under function category Engineering.

User Defined Functions

User defined functions are written in the Visual Basic for Applications Language. They are entered on a Visual Basic module sheet and are immediately available for use on the spreadsheet. User defined functions may be accessed by use of the **Function Wizard** under function category User Defined.

Example of A User Defined Array Function

User defined function "Quad" is an array function whose arguments are the coefficients of the quadratic (a,b,c)

$$f(x) = ax^2 + bx + c = 0$$

(see Figure 1). The function calculates the two roots of the quadratic (real and imaginary parts) and places them in a 2 x 2 cell array. Note that the internal array name (Arr) is set equal to the name of the function.

To utilize the user defined function on the spreadsheet, a 2 x 2 cell array is selected. Then "=Quad (A1:A3)" is entered into the formula bar. This is followed by pressing **Crtl+Shift+Enter.** The two roots (real part, imaginary part) appear in the pre-selected area of the spreadsheet.

Creating an Add-In

The workbook shown in Figure 1 is an *.xls* file. A workbook can consist of module sheets (with subroutine and functions) alone, spreadsheets alone or a combination of the two. It is the starting point for constituting an add-in. *Figure 2* describes the procedure for creating the add-in from an *.xls* file.

Distribution of Add-Ins

Add-Ins are in the form of compiled code (*.xla* files) which cannot be read by anyone and can't be converted back to a workbook. As a result an *.xla* file can be distributed for use by other users of Excel 7.0 without showing the source code (i.e. the .xls file).

CACHE welcomes contributions of add-ins that will be distributed like other CACHE products. The add-ins can be programs like *Solver* or *Goal Seek* user defined function libraries or source spreadsheets *(.xls)* files.

Currently the EMR Technology Group Add-in Library is available from CACHE. It is described in Figure 3.

References

1. Harris, M. Teach Yourself Visual Basic forApplications in 21 Days. *Sams Publications*, Indianapolis (1994).

2. Webb, J. Special Edition Using Excel Visual Basic for Applications. Second Edition. *Que Corporation*, Indianapolis (1996).

3. Visual Basic User's Guide, Microsoft Excel, Version 5. 0. *Microsoft Corporation* (1993).

4. Frey, D.D. Numerical Simulation of Multicomponent Chromatography Using Spreadsheets. *Chemical Engineering Education*, **24** No. 4,. 204-207 (Fall 1990).

5. Savage, P. E. Spreadsheets for Thermodynamic Instruction. *Chemical Engineering Education,* **29**, No. 4, 262-269 (Fall 1995).

6. Mitchell, B. S. The Use of Spreadsheets in Introductory Statistics and Probability. *Chemical Engineering Education*, **31**, No. 3, 194 -200 (Summer 1997).

7. Sandler, S. I. Spreadsheets for Thermodynamics Instruction - Another Point of View. *Chemical Engineering Education*, **31**, No 1, 18-21 (Winter 1997).

Quad Function

```
Public Function Quad (coef)

'Written by EMR Technology Group 10/3/97
'coef - The Vector of quadratic coefficients

Dim Terml As Double
Dim a As Double
Dim b As Double
Dim c As Double

Dim Arr(1 To 2, 1 To 2)

'Value of b2-4ac

a = coef(l)
b = coef(2)
c = coef(3)

Term1 = b ^ 2 - 4 * a * c

If Term1 > = 0 Then

    Arr(l, 1) = (-b + Sqr(Term1)) / (2 * a)
    Arr(1, 2) = 0
    Arr(2, 1) = (-b - Sqr(Term1)) / (2 * a)
    Arr(2, 2) = 0

Else
    Term2 = Sqr(Abs(Term1))

    If b = 0 Then
      Arr(1, 1) = 0
      Arr (2, 1) = 0
    Else
      Arr(1, 1) = -b / (2 * a)
      Arr(2, 1) = -b / (2 * a)
    End If

      Arr(1, 2) = Term2 / (2 * a)
      Arr(2, 2) = -Term2 / (2 * a)

End If

Quad = Arr

End Function
```

Roots of a Quadratic Equation

Coefficients	Output Array	
1		
0	Real	Imaginary
4	0	2
	0	-2

Figure 1
Spreadsheet Showing the Use of Array Function Quad

Adding an Add-In

1. In Excel open the (Library) file (i.e. .xls) to be the add-in.

2. Click on File...Properties

3. Enter the Title of the file under the Summary Tab. (This will be the name of the add-in that will appear in the Add-Ins window). Click OK.

4. On one of the module sheets click on Tools...Make Add-in. Save the .xla file produced in the same folder where the .xls file exists so the source file and compiled files are together.

   Exit Excel. Say "yes" to the "save changes" message in the window message.

5. Startup Excel. Go to the Tools...Add-ins. Click on **Browse.**

6. Locate the .xla file. Click OK.

   The Add-Ins List now contains the name of the add-in. Click OK.

   Check if you want it loaded. Note the functions are available in the function Wizard list under User Defined.

Deleting an Add-In

1. Delete the .xla file (say using Window's Explorer).

2. Start Excel. Notice the message that says the .xla file can't be found.

3. Click Tools...Add-Ins.

4. Locate the name of the file to be removed in the list of add-ins. Click on the name.

5. A message will appear "Cannot find add-in...". Delete from list?".

6. Click Yes. Notice the name has been removed. Click OK.

7. The add-in has been deleted.

Figure 2
Entering and Deleting Add-Ins

The following is supplied as an *.xla* file

Returns a single result:

Interp	A first and second order Interpolation routine
Trapz	An integration routine using the trapezoidal rule
Romberg	An integration routine using the Romberg algorithm

Returns array:

Cubic	Returns all the roots of a cubic equation

The following is supplied as *.xls* file

Rk4a	A fourth order Runge-Kutta routine for up to 5 simultaneous differential equations
ffff1...ffff2	Dummy routines for the right hand sides of Rk4a

Figure 3
EMR Technology Group Add-In Library

New Version of GAMS
Now available from CACHE for Case Study no. 6

GAMS is an acronym that stands for General Algebraic Modeling System, a high level Computer programming language for modeling and solving optimization problems - linear, nonlinear, and mixed integer. It is especially useful for handling large, complex, "one of a kind" problems, which may require many revisions of the model to get the formulation right. GAMS enables you to model problems in a natural way, so that you can easily change your formulation - even convert a model from linear to nonlinear with little trouble.

GAMS was developed primarily by optimization experts Dr. Anthony Brooke and Dr. Alexander Meeraus, formerly of The World Bank. Their goal was to create a powerful but easy-to-use computer programming language that would greatly simplify the modeler's task of formulating and solving complex optimization problems. Recognizing the excellence of GAMS, the Computer Science Technical Section of the Operations Research Society of America awarded its 1987 prize to The World Bank's GAMS development team. Previous versions of GAMS are widely used by academic institutions and industry around the world.

Documentation that accompanies the CD ROM containing the software explains in detail with examples how to make best use of the several algorithms available. Some of the well known codes are MINOS, CONOPT (two versions), DICOPT (for mixed integer problems), OLS (an IBM code), and MILES (for systems of nonlinear equations). CACHE provides a code for PCs running under DOS, Windows 3.1, Windows 95, and Windows NT.

GAMS is designed to use machine resources in a flexible way, and acquires memory as needed to store your data structures. Therefore, it is not possible to specify precise limits for "what will fit". There are some fixed limits built into GAMS and the solvers, but they are large and generally will not interfere with the user.

GAMS software comes with a 286 page manual *GAMS: A User's Guide*, written by the principal authors of GAMS, along with *GAMS - The Solver Manuals* that provides full documentation of the GAMS programming language and solvers: 18 chapters, 6 appendices, glossary, bibliography, and index.

Also included in the manual is an in-depth but easy-to-follow tutorial, which covers the major features of GAMS, using examples from an actual model that comes with the software.

This new version of GAMS is now available from the CACHE office. The cost for Process Design Case Study No. 6, along with GAMS: A User's Guide, and GAMS - The Solver Manuals, and a CD-ROM is $65 per CACHE supporting departments, and $100 per non-CACHE supporting departments.

For more information on GAMS please refer to CACHE web site http://www.che.utexas.edu/cache

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Simulation Sciences

ANNOUNCEMENTS

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.

For more updated information visit the FOCAPO98 web site at: http://unitflops.ecn.purdue.edu/FOCAPO98

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

Program Information

Session	Time	Session Chair	Speakers
Opening Session	Sunday evening	G. Blau Dow Elanco J. Pekny Purdue University	L. Smarr National Computation Science Alliance
Key Note Session	Monday morning	G. Stephanopoulous Massachusetts Institute of Technology	L. Koppel Aspen Technology Y. Natori Mitsubishu Kasei Corp. W. Marquardt Aachen Technical Univ.
Plant Wide Optimization	Monday evening	L. Biegler Carnegie Mellon Univ.	J. Perkins University of London H. DeMeyer Bayer Antwerpen N.V.
Pilot Plant/Market Development Plants	Tuesday morning	P. Basu Searle	S. Macchietto University of London H. Patino Adolph Coors Company
Emerging and High Growth Processes	Tuesday evening	K.S. Chang Pohang University	E. Eagan Motorola
Planning and Scheduling	Wednesday morning	D. Smith Dupont	G. Reklaitis Purdue University
Environmental Issues	Wednesday evening	S. Hasebe Kototo University	G. McRae Massachusetts Institute of Technology H. Kohlbrand Dow Chemical Company
Next Generation Enabling Technology and Deployment Issues	Thursday morning	B. McGarvey Eli Lilly and Company	G. Blau/K. Kuenker Dow Elanco M. Ramage Mobil Oil Corporation

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Program Information

Session	Time	Session Chair	Speakers
Product Integrity/Quality	Friday morning		J. McGregor McMaster University F. Becker Abbott Laboratories
Closing Session	Friday morning		G. Stephanopoulos Massachusetts Institute of Technology
Contributed (Poster) Session	Thursday afternoon		
Vendor Session	Monday, Tuesday, Wednesday afternoon		

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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://unitflops.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:

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CHME 112
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Chemical Process Control - V
Proceedings
Now available from AIChE

A collection of peer-reviewed and edited presentations from the 1996 Chemical Process Control Conference (CPC), held in Tahoe City, California, Chemical Process Control-V offers and assessment of the growth and development of process control in the chemical industries over the last 20 years, as well as the most promising research areas to pursue in the years ahead. The book includes five papers assessing the current status of computer-aided process control in specific industry segments - including food processing, pulping and papermaking, and microelectronics - as well as new and emerging technologies and applications in adaptive and non-linear control, impact of computer science, and predictive control.

A section looking back at past - and ahead to future - research directions, and featuring a paper entitled "CPC-I - CPC V: 20 Years of Process Control Research," and 22 "contributed papers" on subjects ranging from process modeling to the industrial-scale use of neural networks, round out the volume.

Edited by
Jeffrey Kantor, Carlos Garcia, and Brice Carnahan
Available from AIChE office
$64 for North American members
$88 for other members.

Computers in Chemical Engineering Education
Now available from CACHE office

Edited by Brice Carnahan

20 papers by prominent chemical engineering faculty covering a wide range of subjects, from the impact of computing in individual undergraduate chemical engineering courses, to more general topics such as accreditation, multi-media instruction, numerical software, laboratory automation, and the Internet and World Wide Web. The papers are written from the perspective of past computing developments, present activities, and future directions in chemical engineering education.

Table of contents

This book is now availabe from the CACHE office at a cost of $15.00.

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Model Predictive Control Toolbox (CACHE Tools) Manual and 3.5″ PC disk		$160	$250	
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