

CACHE NEWS

NEWS ABOUT COMPUTERS
IN CHEMICAL ENGINEERING
EDUCATION

No. 36

Spring 1993



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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CACHE NEWS

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

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Multimedia Instructional Modules for the Chemical Engineering Laboratory

CACHE is pleased to announce the availability of the results Purdue-Industry collaboration in developing instructional materials for the typical senior course in Chemical Engineering Laboratory. Although the modules were originally intended for use in the senior laboratory, they can be adapted for use in other courses as well. At Georgia Tech, for example, the Amoco Resid Hydrotreater simulation has been used as part of a course in reactor design. Four companies participated in the preparation of the materials as listed in Table 1.

Table 1 Materials Available

| | |
|-------------------|--------------------------------------|
| Amoco | Resid hydrodesulfurization |
| Dow Chemical | Latex emulsion polymerization |
| Mobil | Catalytic reforming |
| Tennessee Eastman | Methyl acetate reactive distillation |

Each group of materials consists of a video tape to show the actual process, a disk containing computer programs to simulate the process, and a set of written materials. The computer programs run on a Sun workstation, and make use of the IMSL libraries. They should be portable to any system running under UNIX and supporting X Windows.

At Purdue, the materials were used as part of the laboratory course as follows. Students worked in groups of three designed as (a) a group leader, (b) an experimentalist, and (c) a design engineer. Each group worked on three month-long projects during the semester. Table 2 shows how the eight three-hour lab periods were allotted to each project.

Table 2 - Lab Schedule

| Week | Period | Activity |
|------|--------|----------------------------------|
| | | Orientation and video plant tour |
| I | 1 | Planning |
| | 2 | Planning/Planning Conference |
| II | 3 | Experiments |
| | 4 | Experiments |
| III | 5 | Experiments |
| | 6 | Experiments/Oral Progress Report |
| IV | 7 | Follow-up problem |
| | 8 | Follow-up problem |

A final report was due one week after Period 8.

Before the first scheduled lab period, the students attended an orientation meeting with the instructor, who answered general questions about the process, the simulation, and the lab. They received a detailed written description of the process, including their initial assignment letter, and they viewed the video plant tour. In keeping with the attempt to provide a sense of realism in the project, the students were given their assignments on official company stationery.

As seen in Table 2, the first two lab periods were spent in preparing a detailed plan of attack. Before students were permitted to begin taking data, they had to present their experimental plan to the instructor in a planning conference. The purpose of the planning conference was twofold: to ensure that the students understood what they were supposed to be doing, and to give them practice in explaining technical concepts.

Once the students demonstrated to the instructor's satisfaction that they were ready to begin their experiments, they were shown how to use the simulator. The programs are designed to be easy to use, even for students having no previous experience with Sun computers.

Once the students finished taking data for the initial assignment, they received a second assignment letter, again on official company stationery. The follow-up problem typically required that they use the data they obtained to perform some useful task such as to recommend a startup procedure, or to explain how to make modifications to the current process equipment. During the sixth lab period, the group leader presented a 15-minute oral progress report to an audience of professors and students. His or her report was videotaped and critiqued in private. The instructor plays four important roles in the course:

- (1) *Mother Nature* - sets the mean values and random variability of all parameters used in the simulation.
- (2) *Boss* - receives reports from the group.
- (3) *Consultant* - helps with specific technical questions, but charges a fee that must be paid from the budget.
- (4) *Instructor* - assigns the grades.

The initial price for each set of materials is \$200, and the annual fee for continued use of the materials is \$25. They may be ordered from CACHE on the order form in this issue.

Microcomputer Chemical Engineering Programs

Developed by Professors

Edited by Bruce A. Finlayson

Have you wondered what microcomputer programs are being used in other chemical engineering curricula? This column provides a mechanism for University professors to let others know about the programs they've developed and are willing to share on some basis.

The program should be described by a 250 word description, machine requirements, and ordering information. These programs should be ready to be shipped out the door, and should have been tested by students at more than one University. It would be helpful if the specific Chemical Engineering course were identified in which the program is useful. The programs will not be reviewed by Professor Finlayson, nor will they be certified by CACHE.

In order to edit the column efficiently, the submissions must be made to Finlayson via BITNET, address FINLAYSON@MAX or on a diskette in ASCII. He will acknowledge receipt of the submission via BITNET and will send the edited column to the CACHE office via BITNET. Letters cannot be accepted.

The column can only be successful if professors submit their write-ups. Let us hear from you!

PICLES: Process Identification and Control Laboratory Experiment Simulator

Prof. Douglas J. Cooper
University of Connecticut

PICLES is an easy-to-use simulator that runs on IBM PC compatible computers to provide real-world experience to those studying process dynamics and control. PICLES is not a control system design package. Rather, this teaching tool, designed specifically for academic and short course use, provides the realistic processes for students to practice upon.

Students can select one of the PICLES processes and manipulate the input variables to obtain pulse or step test data for identification, just as they would on a real process. After performing an identification analysis using the data, students can then design and implement a PID controller to obtain a visual appreciation for the relationship between initial design methods and resulting controller performance.

The available processes include nonlinear behaviors so, students can learn how to compromise controller tuning to maintain stability over a range of nonlinear operation. A "design your own process" facility lets students study, for example, how model order affects controller stability.

There are processes with and without dead time,

noisy and quiescent processes, and integrating process, a process with a negative steady state gain, one that has a nonminimum phase disturbance response, and a multivariable process. PICLES lets students visually appreciate the implications for controller design.

The available controllers are all PID, and the menus make it is easy to compare P-only, PI, PD and PID control modes. Students can compare PI velocity mode with PI position mode, and the difference in performance for derivative on measurement versus derivative on controller error. The Smith predictor lets them learn the benefits of model-based dead time compensation and the feed forward element lets them learn about model-based disturbance compensation. Decouplers enable a study on model-based reduction of controller interactions for multivariable applications. CACHE will shortly be distributing PICLES.

More information can be obtained from:

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EZPlot, XY - Turbo Pascal Units (Libraries) for developing graphical Chemical Engineering Applications.

Dr. James P. Henley Jr.
Auburn University

EZPlot is a graphics unit for plotting functions and data (a unit is like a subroutine library, but much more powerful). XY is a unit for fitting experimental data. EZPlot was developed as a simple, yet powerful tool for visualizing two dimensional numeric data, functions and calculations, and is used in the freshman Chemical Engineering computer course at Auburn. Students quickly learn to write Turbo Pascal programs to graph functions and data. Programs written in Turbo Pascal using the EZPlot unit will run on any IBM compatible computer with CGA, MCGA, EGA, or VGA graphics systems.

XY was developed for binary vapor liquid equilibrium calculations in Unit Operations and Thermo II. The primary procedure in the XY unit is called fit_data and is called in one statement:

```
fit_data('ethanol.dat');
```

The procedure opens the data file "ethanol.dat", does a curve fit of the data, and produces two functions, Xe(y) and Ye(x). In a McCabe Thiele Distillation program, for example, the equilibrium curve, Ye(x) can be drawn by the EZPlot procedure draw:

```
draw(Ye);
```

And in the stage to stage calculations, each time the vapor composition (x) needs to be calculated from the vapor composition (y) on the same tray, the Xe function can be called:

```
x:=Xe(y);
```

When used together, EZPlot and XY allow a wide range of Chemical Engineering Problems to be solved with very short Turbo Pascal Programs. For example, a program that does a graphical McCabe Thiele solution using experimental VLE data is only 70 lines. Other programs written by the author using these units include graphing partial molar properties, liquid liquid extraction, multi-stage batch distillation, VLE diagrams from Benedict-Webb-Rubin, Redlich-Kwong, Wilson, Van Laars, and Margules.

More information can be obtained from:

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UC SIGNAL: Graphical Configuration of Multiloop Control System Signals

Prof. Alan Foss

Students can quickly "sketch" links between measured and manipulated variables, insert controllers and other system elements, and set tuning parameters for controllers, feedforward elements, and decouplers. Their system structure is overlaid automatically on the screen on top of a process diagram prepared by the instructor. System building is accomplished easily through mouse-directed commands to make links, to insert, move or remove elements, to interrogate connectivity, and to display and/or modify parameters associated with

process elements. Control systems can be configured both for laboratory apparatus and process simulations. The completed system is saved in a file and loaded into our real-time control system package UC ONLINE (see following listing).

A student tutorial, an instructor reference, and sample process diagrams are included. Phone and e-mail technical support is provided. A description of the program features and its use in process control education appeared in Chemical Engineering Education 25, 126 (1991).

Equipment needed: PC/AT or faster.
640k RAM.
EGA or better color display.
mouse.

North American academic departmental site license: \$500.

A demonstration diskette is available. Address inquiries to:

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UC ONLINE - version 2.1: Real-Time Multiloop Control System

Prof. Alan Foss

Almost any imaginable multiloop control system can be placed in operation on laboratory apparatus or simulated processes with this easily learned PC-based computer program. Multiloop feedback, feedforward, and decoupling are easily accomplished. So too are gain schedulers, cascades, overrides, and variable structure systems. System elements at the user's disposal are PID controllers (both velocity and position algorithms), summers, multipliers, dividers, square roots, high- and low-selects, delays, lead-lags, ramps, and sinusoids. All may be speedily incorporated into a full control system through use of our interactive graphics program UC SIGNAL (see preceding listing).

Process simulations and custom modules can be written in Microsoft (tm) Fortran and/or C and linked with the program object modules. A distillation column simulation is available as a separate license.

New features in this version include a screen displaying

controller variables and status in a graphical format. One can now bound the rate of change of the output of a controller. Panel displays of system element parameters have been enhanced. Sinusoidal, ramp, and dead-time variables have been added. Controllers now incorporate an audible alarm feature. Datalogging to disk file at user selected intervals has been added. Simulations can now be run at accelerated rates for rapid evaluation of control system performance.

A student tutorial, a user's guide, and an instructor's reference are included. We provide technical support for this product by telephone and/or by electronic mail.

This and earlier versions have been distributed to some 45 institutions worldwide.

Equipment needed: same as for UC SIGNAL (see preceding listing except no mouse is required).

North American academic departmental site license: \$800.

A demonstration diskette detailing the major features is available.

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The following programs have been listed in prior editions of the CACHE News.

1. Vapor compression refrigeration cycle, No. 24 and 25 Stanley Sandler, University of Delaware
2. Compression of an ideal gas, No. 24 and 25, Stanley Sandler, University of Delaware
3. Computer Aided Analysis for Process Systems, No. 24 and 25, Ted Cadman, University of Maryland
4. Discounted Cash Flow Analysis (and Present Worth), No. 24 and 25, Bruce A. Finlayson, University of Washington
5. Short-cut Distillation and Flash Calculations, No. 24 and 25, Bruce A. Finlayson, University of Washington
6. Convective Diffusion Equation (CDEON), No. 25 and 26,

Bruce A. Finlayson, University of Washington

7. Engineering Plot (ENGNPLOT), No. 25 and 26, Bruce A. Finlayson, University of Washington

8. Educational Software for Teaching Process Dynamics and Control, No. 26 and 27, Andrew Hrymak, McMaster University

9. MIDAS - Microcomputer Integrated Distillation Sequences, No. 26 and 27, Andrew Hrymak, McMaster University

10. A Rigorous Multicomponent Multistage Steady-State Distillation Rating Program, No. 27 and 28, E.C. Roche, Jr., New Jersey Institute of Technology

11. RESIM. A Reactor Design Teaching Tool, No. 27 and 28, B.W. Wojciechowski, Queen's University

12. Real-time Multiloop Computer Control Program. UC ONLINE, No. 27 and 28, by Alan Foss, University of California, Berkeley

13. Real-time Dynamic Distillation Simulation and Relative Gain Program, No. 27 and 28, by Alan Foss, University of California, Berkeley

14. The Kinetics and Selectivity of Consecutive Reactions, No. 29 and 30, by Alvin H. Weiss and Reynold Dodson, Worcester Polytechnic Institute

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17. Optimum Series Bioreactor Design, No. 31 and 32, by Gordon Hill, University of Saskatchewan

18. REACT! A Chemical Equilibrium Calculator, No. 32 and 33, by James A. O'Brien, Yale University

19. BioDesigner, No. 33 and 34, by Demetri Petrides, New Jersey Institute of Technology

20. WILSON - A non-ideal vapour-liquid equilibrium tool, No. 34 and 35, by Dr. R.E. Hayes, University of Alberta

Computer Aided Learning in Chemical Reactor Engineering

By Richard Tanner (Dept. of Chemical and Process Engineering) and
Cliff Beevers (Dept. of Mathematics)
Heriot-Watt University, Riccarton, Edinburgh, Scotland EH14 4AS

INTRODUCTION

A computer aided learning (CAL) system for chemical reactor engineering has been developed at Heriot-Watt University. It is used in parallel with traditional teaching techniques in the introductory course to reactor engineering for chemical engineering undergraduates, in the 3rd year of a 4 year BEng Honours degree. The development is based on software used for a proven system for the teaching of mathematics at Heriot-Watt, the Computer Aided Learning project in Mathematics, (CALM)¹.

The CALM project began in 1985 as part of the Computers in Teaching Initiative set up by the Computer Board for UK Universities. A grant of £125,000 was used to equip a network laboratory of 32 Research Machines 186 microcomputers. Each machine has a megabyte of RAM and can be driven via a file server or used in individual mode via its own disc drive. The CALM software is written in Pascal and it can be easily adapted to new areas. It allows group tutorials or individual revision and there is on-line continuous assessment based on the student's responses to the tutorial questions.

This particular development complements lectures on stoichiometry, chemical kinetics, chemical equilibrium and design of the ideal batch reactor, plug flow reactor (PFR) and continuous stirred tank reactor (CSTR). Octave Levenspiel's "Chemical Reaction Engineering" is the recommended text for the course and the modules are loosely based on material from the first 6 chapters².

STRUCTURE OF SYSTEM

Six reactor engineering modules have been developed to date, each consisting of a theory section and worked examples. The tutorial questions may include material from more than one module.

Theory Section

The system is only available after the students have covered the relevant theory in the lecture course and is used in addition to rather than in place of traditional tutorials. As the students are expected to have lecture notes with them, the theory sections are brief, providing only definitions, important formulae and a summary of the main concepts. At no stage is it necessary for the student to read long sections of text from the screen.

As an example, the theory section for the CSTR module consists of just four screens; a drawing of the reactor, a description of the idealities assumed, the design equation and the graphical representation of this equation. Text is revealed stage by stage on the screen, enlivened by the appropriate use of colour.

Graphics and animation are often used to aid understanding and maintain interest. For instance Figure 1 is the graphical representation of the CSTR design equation mentioned above. The graph is slowly plotted on the screen. After a key action from the student, the rectangular block is gradually drawn and shaded in to demonstrate the graphical design method.

Another example of the use of animation is from the theory section for batch reactors, to demonstrate their mode of operation. In a representation of the reactor, the liquid level slowly rises until the reactor is full. After a response from the student, a comment on the screen explains that the reaction is complete and the liquid level falls until the reactor is empty.

Worked Examples

A well structured worked example has the dual role of clarifying the theory and helping to develop a good problem solving technique. Hopefully the students will take the same care in presenting their answers in written examinations. CAL comes into its own here as it allows the student to control the rate at which the solution is presented. This is demonstrated by Figures 2 and 3, two successive screens from a worked example in the stoichiometry module. A key response is required from the student to move on from one screen to the next.

It is important that the question remains highlighted at the top of the screen throughout the solution for the student to refer to. Note that all equations used are shown in algebraic form before the data is entered, to help reinforce the theory. The use of colour allows significant results to be highlighted, such as the calculated concentrations in Figures 2 and 3.

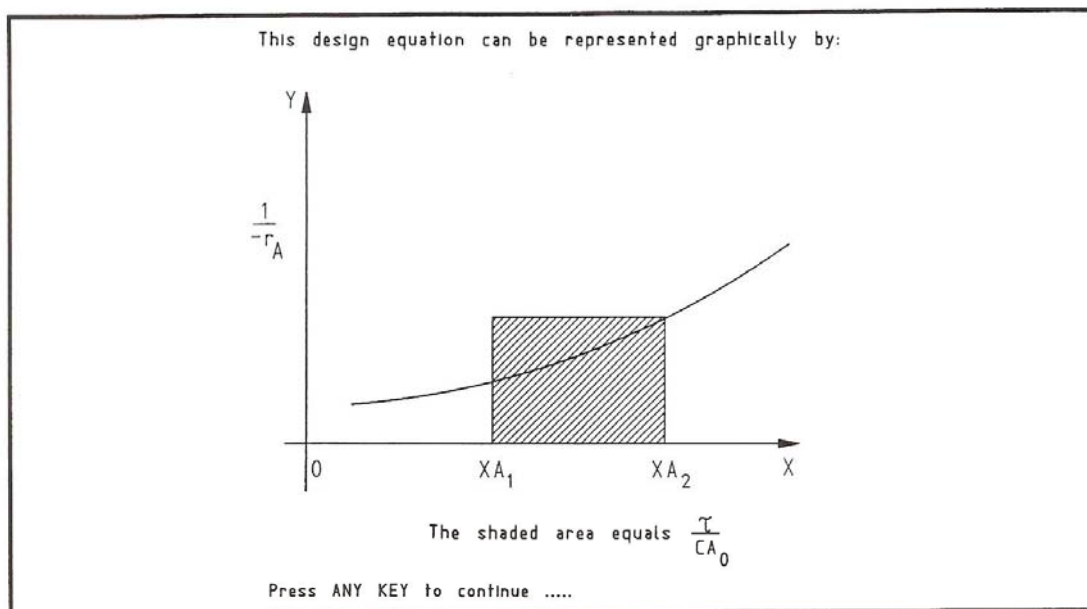


Figure 1: Graphical Representation of CSTR Design Equation

WORKED EXAMPLE 1

Consider the constant volume reaction $A + 2B \rightarrow C + 2D$
 $CA_0 = 4 \text{ kmole/m}^3$, $CB_0 = 10 \text{ kmole/m}^3$, $CC_0 = 1 \text{ kmole/m}^3$, $CD_0 = 0$.
 Find final concentrations of A,B,C & D if 50% of A reacts.

final concentration of B = $CB_0 - (b/a) \cdot CA_0 \cdot XA$
 $= 10 - (2/1) \cdot 4 \cdot 0.5$
 $= 6 \text{ kmole/m}^3$

Press ANY KEY to continue

Figure 2: First Screen from Worked Example on Stoichiometry

WORKED EXAMPLE 1

Consider the constant volume reaction $A + 2B \rightarrow C + 2D$
 $CA_0 = 4 \text{ kmole/m}^3$, $CB_0 = 10 \text{ kmole/m}^3$, $CC_0 = 1 \text{ kmole/m}^3$, $CD_0 = 0$.
 Find final concentrations of A,B,C & D if 50% of A reacts.

If 50% of A reacts, $XA = 0.5$
 final concentration of A = $CA_0 \cdot (1 - XA)$
 $= 4 \cdot (1 - 0.5)$
 $= 2 \text{ kmole/m}^3$

Press ANY KEY to continue

Figure 3: Second Screen from Worked Example on Stoichiometry

Tutorial Questions

Figure 4 shows the final screen from a tutorial question concerning two continuous flow reactors in series:

QUESTION: 7

$A \rightarrow R$

100m³/hr of a 0.5 kmole/m³ solution of A is to be processed in a CSTR and PFR in series.

PFR volume=100m³, CSTR volume=200m³, $r_A = -8CA^2$ kmole/m³ hr.

We want to see how the order of reactors affects conversion.

You will now be asked to input your answer(s). 6 part(s)

| | |
|---|---|
| What is the space time for the CSTR (hr)? 2 | ✓ |
| What is the space time for the PFR (hr)? 1 | ✓ |
| With PFR first, what is intermediate conversion(X)? 80 | ✓ |
| With PFR first, what is final conversion(X)? 89.2 | ✓ |
| With CSTR first, what is intermediate conversion(X)? 70 | ✓ |
| With CSTR first, what is final conversion(X)? 83 | ✗ |

CORRECT ANSWER(S): 2, 1, 80, 89.2, 70, 86.4

YOUR SCORE for this question: 5 out of a possible 6

Press ANY KEY to continue

Figure 4: Tutorial question on Continuous Flow Reactors

The question is quite complex, requiring an understanding of the PFR and the CSTR, but the student is assisted by the careful division of the question into relatively simple steps, such as the calculation of space times and intermediate conversions in this example.

Splitting the question in this way once again helps to develop problem solving skills. The subsequent part of the question only appears on the screen after the student has attempted the previous one. A great deal of thought is required in selecting sufficiently complex problems and in subdividing them.

Each question can be attempted at three levels of difficulty. The simplest level gives the correct answer for each stage immediately the student has made an attempt. The intermediate one marks the attempt without correcting it if wrong, as in Figure 4. At the most difficult level, the marking is carried out after the question has been completed.

Figure 4 shows that graphics can be effectively used to clarify the question. Note also that although the required answers in this example are numerical, algebraic ones can be programmed - these can prove to be a greater test of the student.

STUDENT FEEDBACK

Individual students have used the system as well as su-

pervised classes of up to twenty in the CALM laboratory. In order to assess its effectiveness, students using it have completed a questionnaire and the feedback has been very positive. The general opinion is that it serves its intended role as a backup to existing teaching methods extremely well and that it makes the theory become easier to follow, thus resulting in better understanding. A frequent comment is that a teaching aid of this type increases interest in the subject, leading to a greater willingness to study.

The development has been carried out by final year chemical engineering undergraduates as part of their degree assessment. As well as enhancing their programming ability, they have gained an increased understanding of the subject matter; designing the programmes was a searching test of their grasp of the theory.

FUTURE DEVELOPMENTS

It is intended to develop further CAL chemical engineering modules at Heriot-Watt. Within chemical reactor engineering, nonideal flow is a prime candidate as this is a topic that students traditionally have difficulty in understanding. In addition, residence time distributions can be effectively presented using animated graphics.

CAL is also being considered to assist the teaching of first year undergraduate courses such as the introduction to

material balances. Providing a one-to-one learning environment and being available outside normal teaching hours, it can help with the difficult academic transition between school and university.

This system is one of several developments in CAL at Heriot-Watt University. Leading the way is the recently established Institute for Computer Based Learning. This Institute implements computer based learning methods across the whole university curriculum and pursues research into their impact on teaching. A key development is a "classroom of the future" in which the tools being developed will be used and assessed.

This development was made on a Research Machines Nimbus 186 and is limited to use on that machine. Copies are available on disc (requiring approximately 300 kbytes of system memory) from R.K.Tanner at Heriot-Watt University free of charge. Alternatively, an IBM version of the CALM software itself is now available from Dr J.H.Renshaw, Faculty of Mathematical Science, Southampton University, Southampton, United Kingdom.

ACKNOWLEDGEMENTS

The authors would like to thank Graeme Brown and Quentin Kirk who helped to develop the system as part of their undergraduate studies and Maureen Foster for her programming advice.

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Dispersion Diagram—see page 546

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Interactive Computer Graphics: GNUPLOT

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NSW 2006

AUSTRALIA

Abstract

GNUPLOT can quickly produce, plots, surface plots and contours. It is interactive with the user and in many cases only a 2 line instruction is required. The development work on GNUPLOT has been done by a body of people working worldwide. It is freely available through E-mail. There are many teaching examples in mathematics, process control and chemical engineering simulation which can interact with GNUPLOT. This paper provides enough information to use GNUPLOT and more.

Introduction

GNUPLOT is a graphical package with the strange name but it is a name to be remembered. It is highly interactive with the user and super friendly. If you have the function $f(x)$ given by equation (1) then you might want to know if there are maxima or minima near the origin.

$$f(x) = e^{\sin^3 x} \quad (1)$$

It is fairly difficult to know the answer to this question without going through the usual gradient analysis. In the following solution the computer identification and prompt is given by,

```
furzer %
```

the GNUPLOT solution consists of only 2 lines

```
furzer % gnuplot
gnuplot > splot exp ((sine (x**3))
```

The graphical output is given in the snapshot of the screen shown in Figure 1. The first line calls GNUPLOT and prints a copyright message then the gnuplot prompt. The instruction after the prompt is the powerful plot instruction followed by the function. The output is almost instantaneous and the location of the maxima and minima can be viewed with ease. This is what is meant by the expression, an interactive graphical package. To quit from GNUPLOT type,

```
gnuplot > q
```

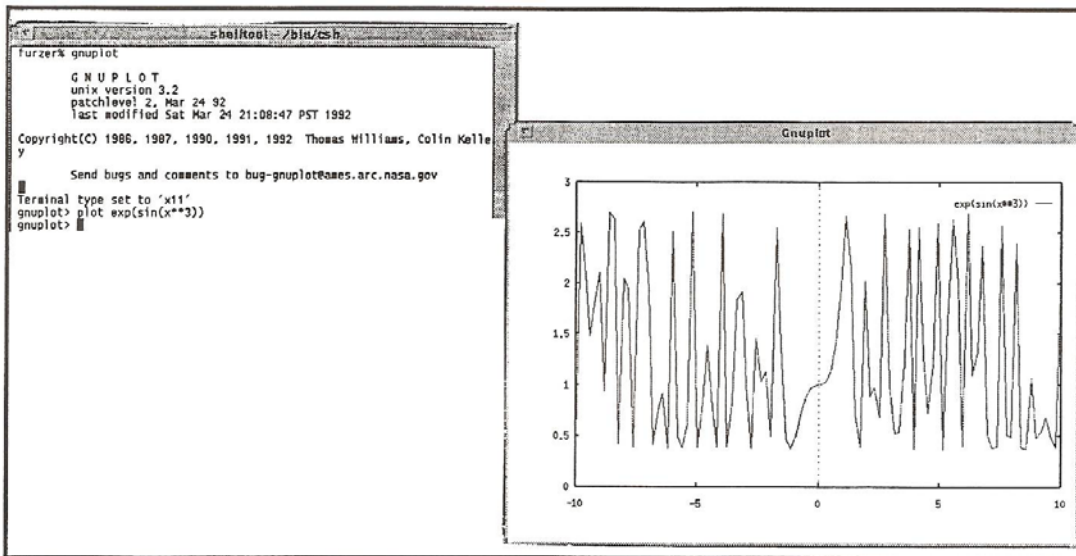


Figure 1: Snapshot of the Sun Sparc 2 Workstation screen

3D Surfaces

GNUPLOT provides a super friendly facility for viewing 3D surfaces. This is particularly important in optimization when searching for maxima or minima. Consider the following function of x and y .

$$f(x,y) = \frac{x^2}{2} - \frac{y^2}{3} \quad (2)$$

The GNUPLOT solution is

```
furzer % gnuplot
gnuplot > splot ((x**2)/2.0 - (y**2)/3.0)
```

The interactive output appears on the screen as is shown in Figure 2. To quit from GNUPLOT type,

```
gnuplot > q
```

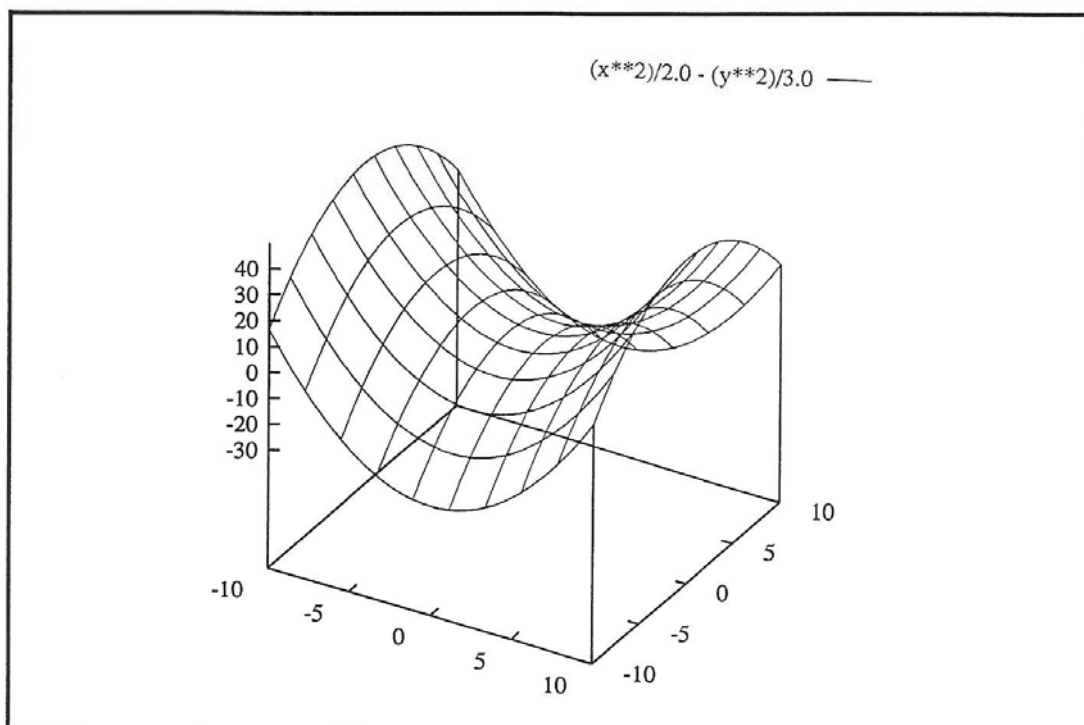


Figure 2: Example of the splot instruction

Contours

GNUPLOT can also provide contours very quickly. The contours of the function $F(x,y)$ given by equation 2 can be seen with the following GNUPLOT solution.

```
furzer % gnuplot
gnuplot > set contour base
gnuplot > splot ((x**2)/2.0 - (y**2)/3.0)
gnuplot > q
```

The interactive output is shown in Figure 3, with the contours projected onto the base of the figure. The two GNUPLOT instructions plot and splot can handle most graphical problems

met by chemical engineers in an interactive manner. Most users of GNUPLOT can stop here, with only the plot and splot instructions.

Computer Systems

The above examples of GNUPLOT were all run on a Sun Sparc 2 Workstation. GNUPLOT has been tested on a wide range of computer systems that include Amiga, AT&T B1, DecStation 5000/200 PXG, IBM PC XT, IBM PC AT, IRIS 4D/70G, IRIS 4D/25G, Next, Pyramid 90X, Sun 3, Sun 4, and Vax 6410. This list is being extended all the time and your computer system is almost certain to be covered by GNUPLOT. It should be noted GNUPLOT operates under a

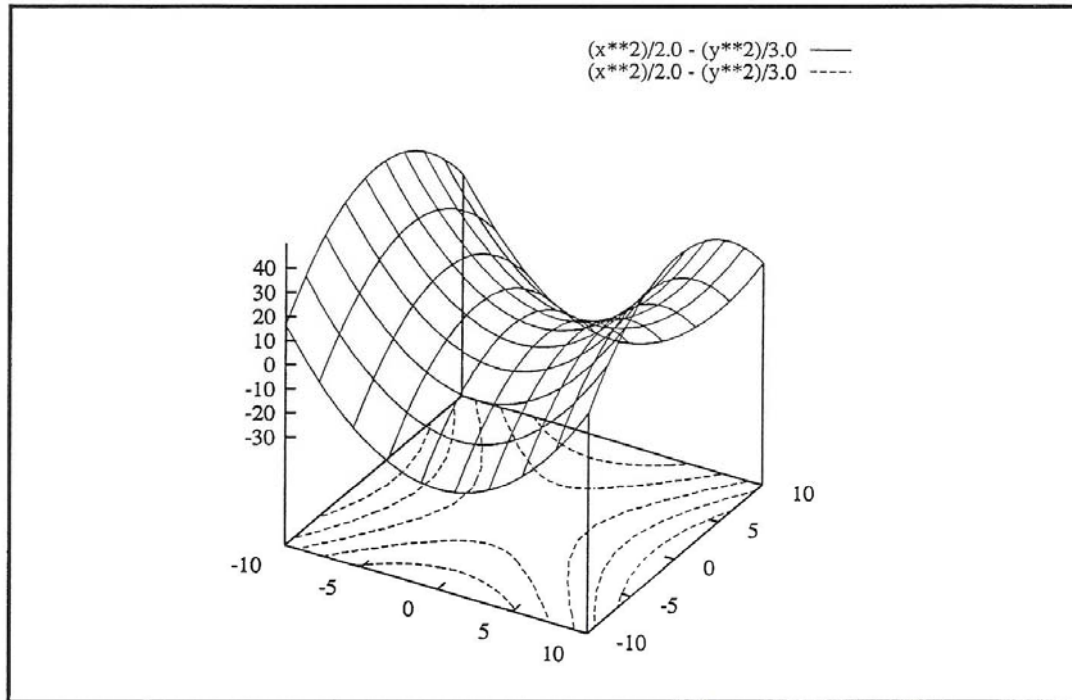


Figure 3: Examples of contours on the base

wide range of operating systems including MSDOS and UNIX. GNUPLOT is copyright by Thomas Williams and Colin Kelley and they have provided permission for use provided the copyright notice shown on Figure 1 is given. A large number of contributors have developed GNUPLOT to Version 3.2 and an updated version is expected soon. This worldwide effort has been by Ed Kubatic, Gershon Elber, Kevin Russo, Alex Woo, Russell Lang, Nick Strobel, Craig Johnston, Michael Schuh, Wolfgang Moeller, Carsten Steger and Rob Cunningham.

There is an X11 version of GNUPLOT which operates under Openwindows. This version is particularly important for high speed workstation. It has been tested on Apollo 400S, Convex C2, Cray 2, Cray Y-MP, IBM RS/6000, NeXT, Sequent Dynix, Sun 3, Sun SPARC, Vax BSD and Vax Ultrix.

Demonstration Packages

GNUPLOT comes with a wide range of demonstration packages to provide straight forward plot and splot examples to more sophisticated examples demonstrating the full range of GNUPLOT. The following demo files come with GNUPLOT, bivariat, contours, controls, electron, errorbar, hidden, param, polar, polardat, simple, surface 1, surface 2, using and world. It is very useful to examine these files and run them with GNUPLOT to see a wide range of examples. To see all the examples, perform the following GNUPLOT instructions after moving to the demo directory.

```
furzer % gnuplot
gnuplot > load "all.demo"
gnuplot > q
```

Improved Plots

Figure 3 shows the surface and contour plots of equation (2). The surface plot contains a 10 x 10 grid which often provides sufficient data to see the surface shape. Due to the twisting of the curved surface, some lines are shown which should be hidden. To improve the figure use,

```
furzer % gnuplot
gnuplot > set isosamples 20
gnuplot > set hidden3d
gnuplot > splot ((x**2)/2.0 - (y**2)/3.0)
gnuplot > q
```

The output showing the improved quality of the surface is shown in Figure 4. The surface is a hyperbolic paraboloid with a saddle point minimum.

GNUPLOT has considerable computing power and the difference equation give by May (1976) can be readily solved. May was examining the bifurcating hierarchy of stable cycles leading to random fluctuations of the following equation.

$$x_{i+1} = ax_i(1 - x_i) \quad (3)$$

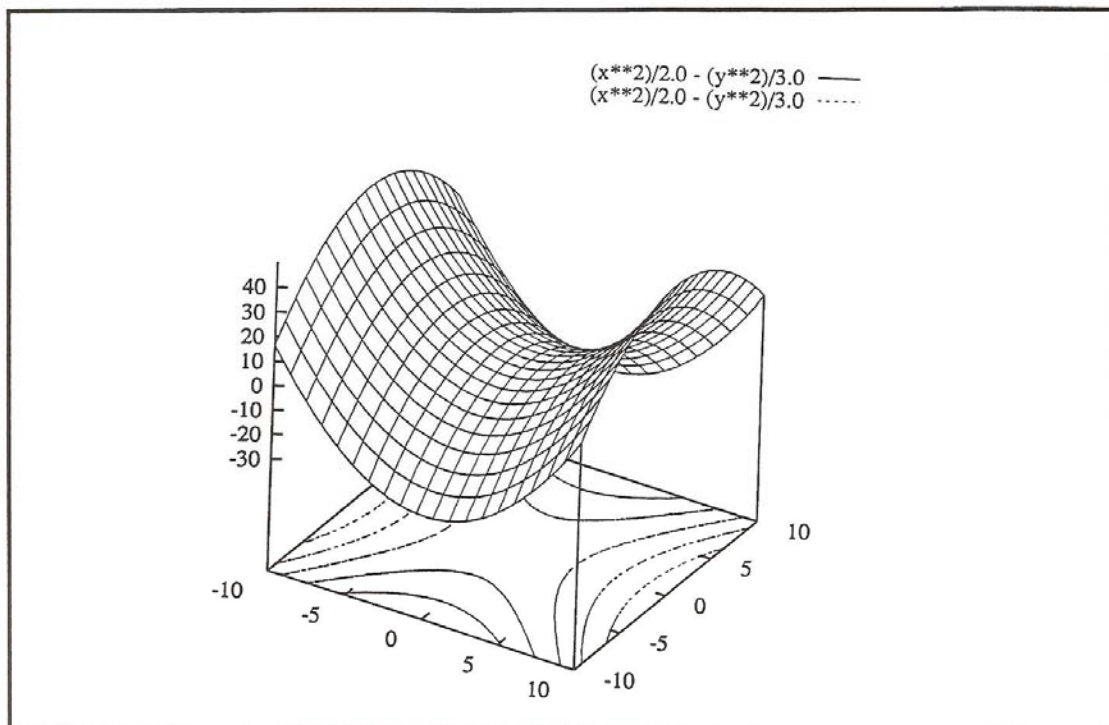


Figure 4: Example of the 20 x 20 grid and hidden line removal

He found there was a stable cycle of period 3 and was able to demonstrate this phenomena by the intersections of the relationship between x_{i+3} and x_i when $a = 3.9$ and a line of slope 1 passing through the origin. The GNUPLOT solution is given in the x range [0:1] by,

```
furzer % gnuplot
gnuplot > a = 3.9
gnuplot > one (x) = a * x * (1-x)
gnuplot > two (x) = a * one(x) * (1 - one (x))
gnuplot > three (x) = a * two(x) * (1 - two (x))
gnuplot > plot [0:1] three (x), x with lines
gnuplot > q
```

The intersections are shown on the output in Figure 5.

GNUPLOT Installation

GNUPLOT would normally be installed on your computer system by the resident UNIX guru. This section may contain some unfamiliar instructions for readers not familiar with UNIX. E-mail information on GNUPLOT can be obtained from,

info-gnuplot@ames.arc.nasa.gov

the present tarred version of GNUPLOT is

gnuplot3.2.tar.Z

This is available from sources in North America, Europe, Australia and elsewhere, see info-gnuplot. Files are transmitted worldwide through the ftp facility. There are deposited in the following directory.

/usr/local/src/gnuplot

These files contain a number of README files which should be read. README.install contains compile instructions on the C compiler and the Makefile. The Makefile is modified to suit your computer system. The installation provides man pages and a help facility. GNUPLOT documentation is in the docs directory and can be supplied interactively when an error is made, through the man pages or as a printed document. There is a considerable amount of work required in this installation but it is worth it.

GNUPLOT Environment

The UNIX C shell Information is kept in the file.cshrc. The following alias is helpful.

alias g gnuplot

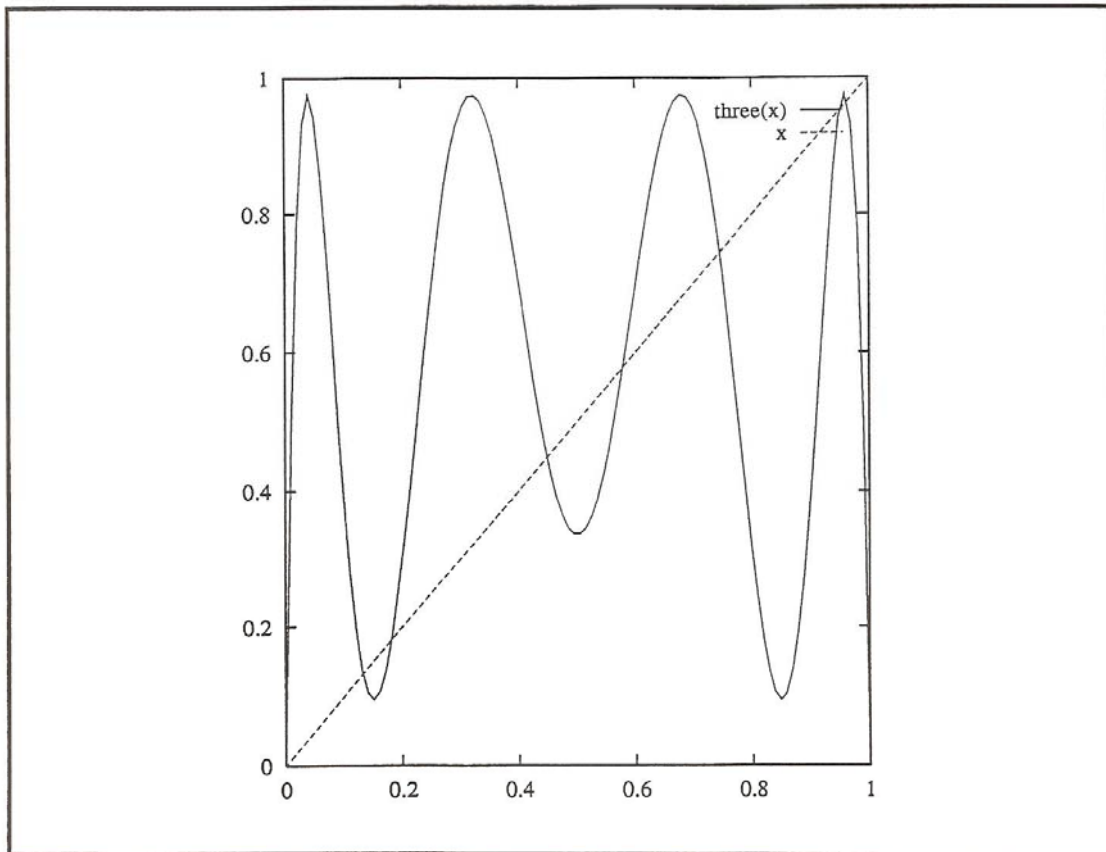


Figure 5: May's example of period 3

The call to GNUPLOT is simplified to,

```
furzer % g
```

The GNUPLOT documentation runs to 40 pages and no attempt will be made here to describe all the features. For presentation of figures for printing quality in a journal it is possible to alter the GNUPLOT environment through the set instruction to add a title, an x label, a y label and other tics and arrows. Two set instructions have already been used, set isosamples and set hidden3d. The set size instruction is useful in producing a square figure.

```
set size 0.66, 1
```

After a plot or splot run it is possible to preserve the graph as a postscript file for printing on a laser printer. There terminal is set to postscript, the output filename given and the graph is replotted by,

```
gnuplot > set term postscript portrait "Times-Roman" 14
```

```
gnuplot > set size 0.66, 1
gnuplot > set output "files.ps"
gnuplot > replot
gnuplot > q
```

To print the figure with a Sun Sparc2 Workstation use,

```
pl file.ps
```

It is possible to preserve all the previous GNUPLOT instructions before quitting. This is done through the save instruction. In the previous example to save everything on a file use,

```
gnuplot > replot
gnuplot > save "file.gnu"
gnuplot > q
```

To rerun this example at a later GNUPLOT session use the load instruction,

```
furzer % g
```

```
gnuplot > load "file.gnu"  
gnuplot > g
```

No output appears on the screen, it is directed to file, "file.ps".

If a large computer program in another language such as Fortran generates a file containing x, y information, then this file can be loaded into GNUPLOT to generate a plot (or splot with x, y, z info) output. For example the following data file contains x, y data.

```
Datafile (cee6.dat)  
x      y  
1      1  
2      2.2  
3      3.3  
4      4.4  
5      5.5
```

The GNUPLOT session is as follows,

```
furzer % g  
gnuplot > plot "cee6.dat" with linespoints  
gnuplot > set size 0.66, 1  
gnuplot > set xlabel "x axis"  
gnuplot > set ylabel "y axis"
```

```
gnuplot > set ylabel "y axis"  
gnuplot > set title "Furzer: Data Example"  
gnuplot > set term postscript portrait "Times-Roman" 14  
gnuplot > set output "cee6.ps"  
gnuplot > replot  
gnuplot > save "cee6.gnu"  
gnuplot > q
```

The output is shown in Figure 6.

Conclusion

GNUPLOT is a very useful interactive graphic package which will handle most chemical engineering problems with speed. It has the advantage of permitting changes to the plot on the screen to get it right then outputting to a laser printer. Many examples in chemical engineering courses can be covered by this single graphical package, GNUPLOT.

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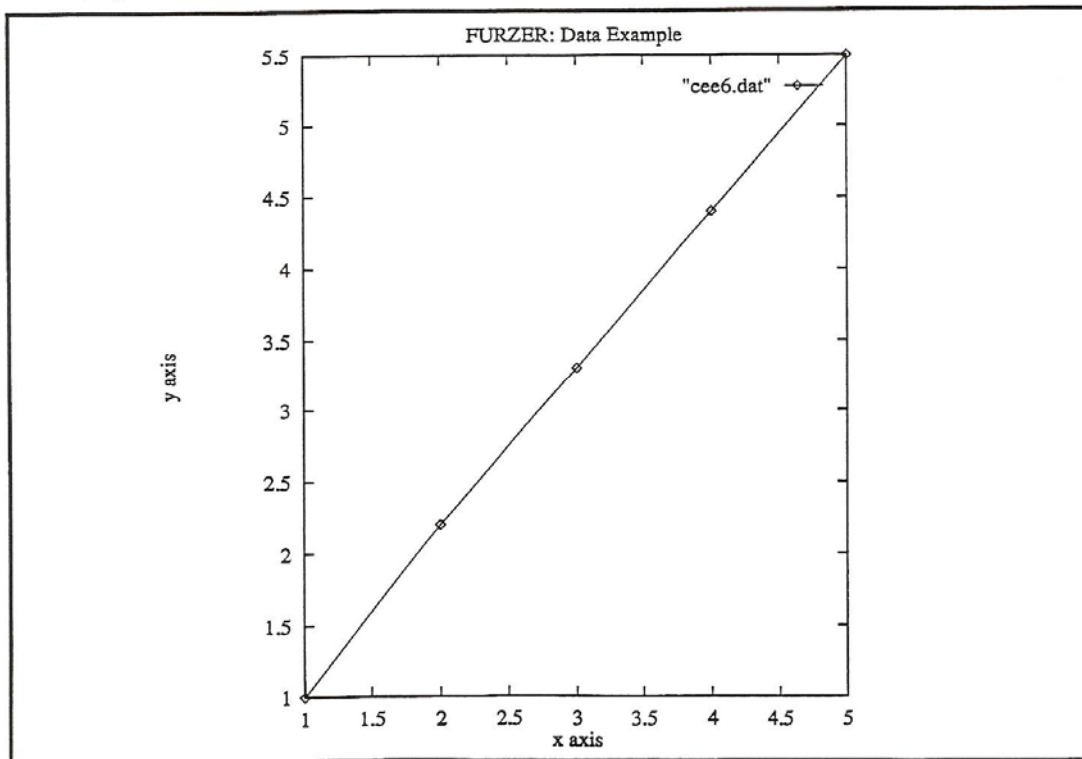


Figure 6: Example of a datafile and labels

DICOF: A Package for Multivariable Controller Design in the Frequency Domain

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NSW 2006

AUSTRALIA

Introduction

DICOF is a set of .m files which run on MATLAB and allows the synthesis/evaluation of controllers for general delayed systems. The set of .m files in DICOF implement the design methodology of Agamennoni et. al. (1985, 1988 and 1992). Figure 1 shows the linear MIMO nominal plant modeled by the transfer matrix $G(s)$, the controller transfer matrix $K(s)$ and the precompensator transfer matrix $E(s)$. In the DICOF context, $K(s)$ notes the ideal controller (the controller that allows to achieve all the performance specifications) and $C(s)$ a reduced order approximation to $K(s)$.

DICOF is particularly oriented to evaluate the controller parameters of a multivariable control scheme that may be directly configured in a Distributed Control System (DCS). This configuration is possible by using standard blocks such as PIDs, delay units and first order low pass filters (lag filters). However, DICOF allows also to synthesize high order controllers, and may be used either with SISO as well as MIMO systems. Delay compensation capability may be easily introduced. If the control system is affected by sluggish disturbances, DICOF allows to tune the controller parameters to introduce a disturbance rejection capability in the control scheme.

DICOF is also a valuable tool for teaching undergraduate and graduate control courses, since it provides and

alternative way to design simple multiloop as well as multivariable robust controllers.

How to use DICOF

Now we will briefly describe how to use DICOF by using two examples. The first one is the following SISO delayed and open loop unstable system

$$g(s) = \frac{0.9 e^{-s}}{s - 0.7}$$

that may be stabilized with a unitary controller $c=1$. Then we will evaluate a delay compensator controller for the stabilized system $g(s)/(1+g(s))$. the second example is the following MIMO system affected by disturbances.

$$G(s) = \begin{bmatrix} \frac{1}{s+1} & \frac{0.5}{s+2} \\ \frac{0.3}{s+2} & \frac{1}{3s+1} \end{bmatrix} \quad D(s) = \begin{bmatrix} \frac{1}{5s+1} & 0 \\ 0 & \frac{1}{5s+1} \end{bmatrix}$$

The following tables summarize the steps to follow using DICOF and the meaning of the output arguments

| Outputs | Meaning |
|---------|--|
| dels: | delay of compensation of each loop noted as θ in fig 1. |
| dens: | denominators of the controller $C(s)$. |
| nums: | numerators of the controller $C(s)$. |
| lagfs: | lag filter to be used in each loop. |
| errs2: | 2-norm of the approximation error. |

| | General steps | Steps for example 1 Stabilized delayed SISO | Steps for example 2 Disturbed MIMO |
|---|---|--|--|
| 1 | Edit a .m file with the plant matrix transfer function | <code>function [f]=plant1(s) g=0.9*exp(-s)/(s-0.7); f=g/(1+g);</code> | <code>function [g]=plant2(s) g=[1/(s+1) 0.5/(s+2)] 0.3/(s+2) 1/(3*s+1)]</code> |
| 2 | Define z with the desired closed loop polynomial of each loop | <code>0.3s+1 >>z=[.3 1];</code> | <code>both loop with 2s+1 >>z=[2 1 2 1];</code> |
| 3 | Define dte with the disturbance time constant to be rejected in each loop | <code>>>dte=[0];</code> | <code>>>dte=[5 5];</code> |
| 4 | For PI controller set lagf =[0] Otherwise, define a vector with possible lag values. | <code>>>lagf=[.2 .4 .6 .8 1];</code> | <code>>>lagf=[1 2 3 4];</code> |
| 5 | Set tdelay =[0] if a delay compensation is not required. Otherwise, define tdelay with possible delays of compensation. | <code>>>tdelay=[.9 .95 1 1.5];</code> | <code>>>tdelay=[0];</code> |
| 6 | Define the order of the controller dl . (1:PI, 2:PID,3,...) | <code>>>dl=2;</code> | <code>>>dl=2;</code> |
| 7 | Define the frequency range of the approximation. fred =1 is the default range of DICOF. fred <1 reduce the final frequency. | <code>>>fred=1.5;</code> | <code>>>fred=1.5;</code> |
| 8 | Use DICOF function | <code>>>[dels,dens,nums,lagfs, errs2]=dicof('plant1',z, dte,lagf,tdelay,dl,fred);</code> | <code>>>[dels,dens,nums,lagfs, errs2]=dicof('plant2',z, dte,lagf,tdelay,dl,fred);</code> |

With **z** and **dte**, and the evaluation of **b** in figure 1 is straightforward. Figures 2-4 show the time simulation for examples 1 and 2. With respect to the second example, an alternative

controller was evaluated by setting **dte**=[0] to show the disturbance rejection effect of the previous controller. The following table summarizes the time simulation experiences.

| Example | Figure | Input | Output |
|---------|--------|---|--|
| 1 | 2 | Unitary step in the reference | Output |
| 2 | 3 | Unitary step in disturbance input 1 at t=0[min.] and a unitary step in input 2 at t=10[min.]. | Output 1 with (----) and without (___) disturbance rejection |
| 2 | 4 | Unitary step in disturbance input 1 at t=0[min.] and a unitary step in input 2 at t=10[min.]. | Output 2 with (----) and without (___) disturbance rejection |

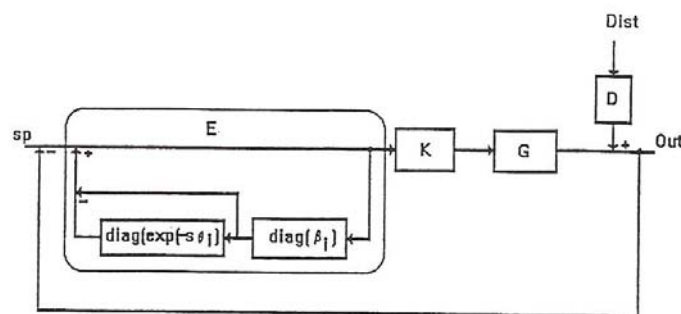


Fig. 1: MIMO DICOV control scheme

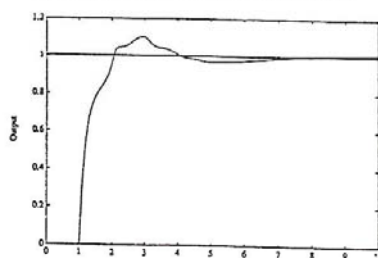


Fig. 2: Example 1

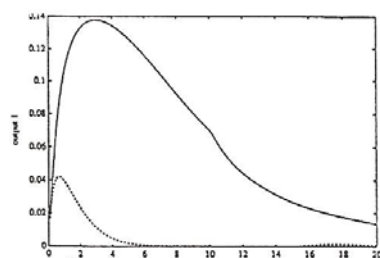


Fig. 3: Example 2
Output 1

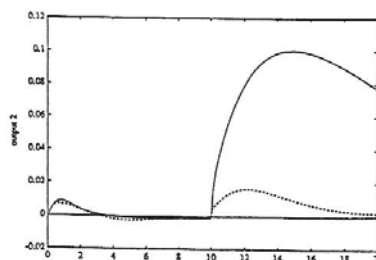


Fig. 4: Example 2
Output 2

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