CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 41 Fall 1995



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.

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

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Picles 4.1 and the Case of the Diabolical Dead Time

By Douglas Cooper, University of Connecticut

Introduction

Meaningful experience in applying textbook theory is an important aspect of the learning process. Such experience is motivating, promotes critical thinking, facilitates understanding of the use and limits of the theory, and better prepares students for the competitive challenges of the professional world. For process dynamics and control, PiclesTM, the Process Identification and Control Loop Explorer System, is a cost effective way to provide this experience.

Picles is IBM PC compatible software now being used in more than a third of the process dynamics and control courses in the U.S. Picles is an easy-to-use training simulator that provides hands-on experience to those studying this often abstract and mathematical subject. Picles contains a series of case studies, animated in color-graphic display, for self-paced or faculty guided learning. Users can manipulate process variables in open loop to obtain pulse, step, sinusoidal or ramped test data. Picles can record this data as printer plots or disk files for process identification and controller design. DigestTM, companion software to Picles, is one package well suited for this identification and design task. After designing a controller, return to Picles and immediately evaluate and improve upon the design for both set point tracking and disturbance rejection.

After a brief review of program features, this article explores one case study possible with Picles. In this case study, Picles' Design a Process, which simulates process dynamics based on user-specified transfer functions, is used to isolate and explore the impact of process dead time on open and closed loop dynamic behavior. This case study also presents the use of the Smith predictor as a model based controller algorithm for dead time compensation. As part of the discussion, Digest's dynamic modeling and controller design capabilities are demonstrated. Note that a host of other studies could be explored using the options available in Picles.

The Picles Case Studies

Previous CACHE News articles describe the Picles processes and present additional case studies [1-3]. The processes available in Picles for investigation include:

One-Input One-Output Case Studies:

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

Ideal Transfer Function Case Study:

Design a Process

Multiple Steady State Case Study:

Jacketed Reactor

Two-Input One-Output Cascade Case Study: Jacketed Reactor

Two-Input Two-Output Multivariable Case Study: Distillation Column

The Picles Controllers

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

Manual Control

P-Only Control

I-Only Control

Velocity PID Control with Derivative on Measurement

Velocity PID Control with Derivative on Error

Position PID Control (no windup protection)

Velocity PID with Smith Predictor

Velocity PID with Feed Forward

Velocity PID with Decouplers Digital Sampled Data Controller

Design a Process

Picles enhances learning of process dynamics and control concepts through "real world" application of theory. Although defining process behavior with ideal transfer functions tends toward the abstract, the Design a Process facility enables specific process behaviors to be isolated and explored. Example behaviors include isolating process order, the impact of lead elements, or in this particular case study, the consequences of dead time on open and closed

As shown in Fig. 1, the Design a Process menu provides separate transfer functions for the process and the load disturbance. This capability permits interesting feed forward controller studies. It is also valuable for exploring how controller design must sometimes balance set point tracking and disturbance rejection performance when the process and disturbance behaviors are different. For each transfer function, a steady state process gain, up to three process

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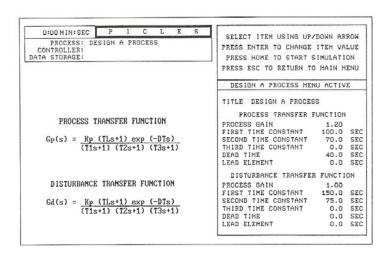


Figure 1 - Design a Process main menu lets user specify both process and disturbance transfer functions

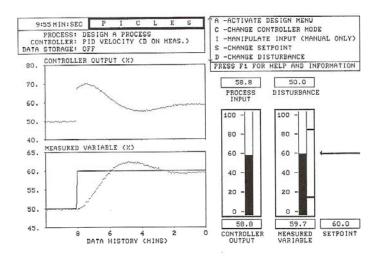


Figure 2 - Animated graphics show both data history plots and error bar displays for manipulated and measured variable

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time constants, a dead time and a lead element can be specified.

After defining the transfer functions and starting execution, Fig. 2 shows the process graphic display animated on the screen. As shown, the display includes both real time data history plots and error bar graphics for the manipulated and controlled variable.

Objective Of This Case Study

In this case study, the impact of dead time on process behavior and controller performance is explored. Specifically, a second order process with no dead time is first defined using Design a Process. Digest is then used to model process dynamics and obtain initial tuning parameters for a PI controller. The controller design criteria for this study is the tracking of set point steps from 50% up to 60% with a 10% peak overshoot ratio and complete settling of dynamics in one cycle of the measured variable. Next, significant dead time is added to the original second order process and the resulting degradation in controller performance is studied. Finally, a model based Smith predictor is designed and implemented to compensate for the process dead time and to restore desirable closed loop performance.

PI Control Without Dead Time

The process chosen here for study is:

$$G_{p}(s) = \frac{Y(s)}{U(s)} = \frac{K_{p}}{(\tau_{p_{1}}s+1)(\tau_{p_{2}}s+1)} = \frac{1.2}{(100s+1)(70s+1)}$$
(1)

where Y(s) is the measured variable and U(s) is the manipulated variable in the Laplace domain. Thus, the process is second order with a steady state gain of 1.2 (unitless) and time constants of 100 seconds and 70 seconds.

The traditional method of approach to feedback controller design as detailed in the popular process control texts is to:

- step or pulse the manipulated variable in open loop (manual mode),
- record the manipulated and measured variable data as the process responds to the step or pulse,
- fit a low order linear dynamic model to this manipulated to measured variable data.
- use the linear dynamic model parameters in one of several popular correlations to obtain initial estimates of controller tuning parameters,
- implement this controller (close the loop) and evaluate its performance in tracking set point changes (disturbance

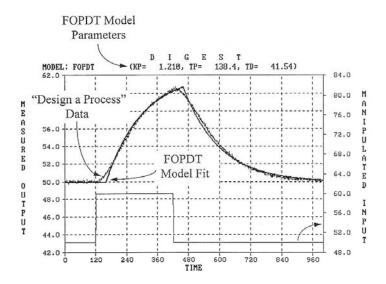


Figure 3 - Digest fits FOPDT model to transfer function data

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rejection is not included in this case study but would normally be evaluated at this point),

 perform a final tuning by trial and error until desired controller performance is obtained.

Following this procedure for the process defined by Eq. 1, a pulse test is performed by stepping the manipulated variable from 50% up to 60%, and five minutes (300 seconds) later, returning it to its original value of 50%. Picles' file storage utility is used to save the data to disk. Digest is then used to fit a low order dynamic model to the data and these model parameter values are used to compute initial controller tuning values.

Digest can import files containing dynamic data from Picles, other software and even from a real plant. The data must be in ASCII tabular form with data columns separated by tabs, commas or spaces. Simple commands are used to mark the manipulated variable data, the measured variable data and the time data. The linear models available in Digest include first order, first order plus dead time (FOPDT), second order and second order plus dead time dynamic forms.

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

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

Fig. 3 shows the Digest fit of a FOPDT model to the dynamic data collected from the pulse test just described. As shown at the top of the figure, the FOPDT model parameters computed by Digest are:

Process Gain, Kp = 1.21 (unitless) Overall Time Constant, $\tau_P = 138.4$ seconds Apparent Dead Time, $\theta = 41.54$ seconds

It is interesting to note that a FOPDT model fit for this second order without dead time process includes a rather significant apparent dead time of 41.54 seconds. This result is appropriate given that, as shown in the figure, a FOPDT dynamic model reasonably approximates the process data.

The dynamic model parameters are now used in correlations to obtain initial estimates for controller tuning. Digest contains a number of correlations, including IMC (internal model control), Cohen-Coon, IAE (integral of absolute error), and ITAE (integral of time weighted absolute error) and will compute the tuning parameters for

a P-Only, PI or PID algorithm at user request. Fig. 4 shows such a computation for the above FOPDT model parameters for a PI controller.

In this case study, IMC controller tuning is chosen. Circled in Fig. 4 are the IMC tuning parameters computed by Digest. Note that Digest recommends a closed loop time constant, τ_C , following the heuristic that τ_C equals $0.1\tau_D$ or 0.8θ , whichever is larger. The user can change this closed loop time constant value and Digest will recompute the IMC parameters.

```
Controller Mode: PI
       Internal Model Control (IMC)
TC (Closed Loop Time Constant) =
Controller Gain
                      1.529
Reset Time
                      138.4
Controller Gain =
                      2.546
                      85.55
Reset Time
       ITAE (for Set Point Changes)
Controller Gain =
                      1.458
                      141.1
Reset Time
      ITAE (for Disturbance Changes)
Controller Gain =
Reset Time
                      90.58
       IAE (for Set Point Changes)
Controller Gain =
                     1.765
                      149.9
Reset Time
      IAE (for Disturbance Changes)
oller Gain = 2.663
Controller Gain =
                      97.20
Reset Time
```

Figure 4 - IMC based PI tuning parameters computed by Digest for the FOPDT parameters of Fig. 3

Thus, Digest recommends the PI tuning parameters:

```
Controller Gain, K_C = 1.529
Reset Time, \tau_I = 138.4 seconds
```

Returning to Picles, the Velocity PID with Derivative on Measurement controller is selected and these tuning values are entered. The derivative time is set to zero, resulting in the desired PI controller form. Note that because derivative time is zero, the Velocity PID with Derivative on Error controller would produce identical results in this case study. Following the design procedure listed previously, the controller is now tested to evaluate its performance.

The capability of the PI controller in tracking step changes in set point is shown in Fig. 5. As shown, for a set point step from 50% up to 60%, the controller achieves the desired controller performance criteria with no trial and error adjustments necessary. That is, the IMC tuned PI controller produces the design peak overshoot ratio of 10% with complete settling in one cycle of the measured variable in about 10 minutes. As read from the plot, rise time for the set point step is about 2.5 minutes.

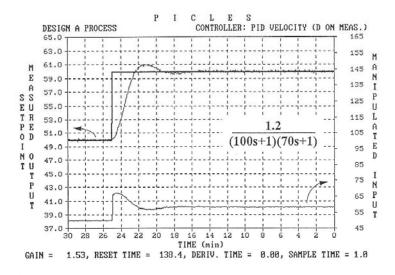


Figure 5 - IMC tuned PI controller produces the design 10% overshoot, complete settling in 10 minutes and a rise time of 2.5 minutes

PI Control With Dead Time

The case study now considers the impact of process dead time. The process transfer function of Eq. 1 is modified with the addition of 40 seconds of dead time to produce the new transfer function:

$$G_{p}(s) = \frac{Y(s)}{U(s)} = \frac{K_{p}e^{-\theta s}}{(\tau_{p1}s + 1)(\tau_{p2}s + 1)} = \frac{1.2e^{-40s}}{(100s + 1)(70s + 1)} \tag{2}$$

To obtain an initial assessment of the impact of dead time on controller performance, the PI tuning parameters used to generate Fig. 5 are retained and the same set point step test is performed. As shown in Fig. 6, the addition of dead time results in seriously degraded performance. The peak overshoot ratio has climbed from its original value of 10% up to about 50%. Complete settling of dynamics has increased from 2.5 minutes up to more than 25 minutes with multiple cycles of the measured variable.

To achieve the design performance criteria of a 10% peak overshoot ratio and complete settling within one cycle of the measured variable, the controller must be detuned (controller tuning must be relaxed). Since the process has been altered to include significant dead time, the most efficient way to determine the new settings is to follow the

identical design procedure just detailed. That is, the transfer function process of Eq. 2 is pulsed in open loop, a FOPDT model is fit to the pulse test data, IMC based PI controller tuning is computed from the FOPDT dynamic model parameters, and controller performance is evaluated in tracking set point steps.

Following this procedure, Digest computes a Kp of 1.22, a τp of 143.1 seconds and a θ of 78.46 seconds. Using the IMC tuning relations, Digest computes a K_C of 0.831 and a τl of 143.1 seconds. As shown in Fig. 7, this tuning produces the design performance criteria of a 10% overshoot ratio and complete settling within one cycle of the measure variable. In this case, settling occurs in 14 minutes rather than the 10 minutes of the no dead time case of Fig. 5. Also, rise time has increased from the previous 2.5 minutes for the no dead time case up to about 4.5 minutes as exhibited in Fig. 7.

Smith Predictor Theory

The addition of significant dead time results in a clear degradation of best achievable controller performance when using a traditional feedback algorithm. A popular method for improving performance in the presence of significant dead time is with a model predictive control (MPC)

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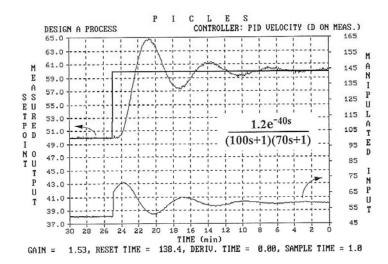


Figure 6 - With the PI tuning of Fig. 5, the added dead time causes a 50% overshoot, complete settling in excess of 25 minutes and a rise time of 2.8 minutes

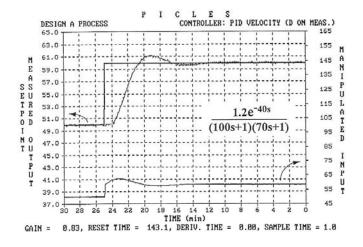


Figure 7 - Detuning the controller produces the design 10% overshoot, but complete settling is now 14 minutes and rise time is 4.5 minutes

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algorithm. MPC algorithms incorporate a dynamic model of the process internal to the architecture of the controller. This internal dynamic model is hereafter referred to as the controller model. The predictive capability of the controller model provides advanced warning of future events which can be exploited to improve, sometimes dramatically, closed loop performance.

The Smith predictor is perhaps the simplest example of MPC (a variant of the Smith predictor can be created using the traditional MPC formulation by choosing a near and far prediction horizon of $\theta/T+1$, a control horizon of 1, and a constant set point profile). To understand the Smith predictor, consider the internal model control architecture illustrated in Fig. 8.

As shown in Fig. 8, the Smith predictor controller model is comprised of an ideal process model block and a dead time model block. Note that Picles provides only a first order dynamic form for the ideal process model block although the general theory permits other model forms to be used. The computational procedure for the Smith predictor is as follows:

 The ideal process model receives the current value of the manipulated variable, U(s), and produces Y_{Ideal}(s), which is a model based prediction of what the measured variable, Y(s), would be if there were no dead time in

- the process (or alternatively, a prediction of what Y(s) will be one dead time into the future).
- 2) $Y_{Ideal}(s)$ is fed into a dead time model where it is stored until θ seconds have passed. At the instant that the $Y_{Ideal}(s)$ is stored, a previously stored $Y_{\theta}(s)$ is released. This $Y_{\theta}(s)$ is the value of $Y_{Ideal}(s)$ which was computed and stored one dead time ago. Hence, $Y_{\theta}(s)$ is a model based prediction of the current value of Y(s)

If the controller model accurately describes the dynamic behavior of the actual process then:.

$$Y_{\Omega}(s) \cong Y(s)$$
 (3)

and

$$Y(s) - Y_{\theta}(s) + Y_{Ideal}(s) \cong Y_{Ideal}(s)$$
 (4)

Thus, the error going to the controller becomes:

$$E^*(s) \equiv Y_{SP}(s) - Y_{Ideal}(s)$$
 (5)

In short, E*(s), the Smith predicted error going to the controller, rather than being the traditional difference between the set point and the measured variable, is

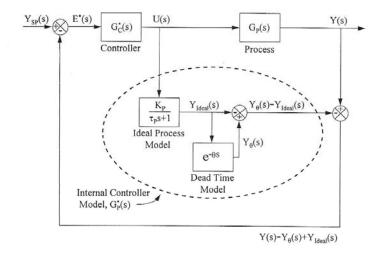


Figure 8 - The Smith predictor controller architecture

approximately the difference between the set point and a prediction of what the measured variable would be if there were no dead time in the process.

Based upon the assumption of Eq. 3, a good match between the controller model predictions and the actual process dynamics is fundamental to the success of the Smith predictor. With a good match, the Smith predictor can dramatically improve controller performance. Be aware, however, that a poor match between the controller model predictions and the actual process dynamics invites disaster, including creating an unstable closed loop system for an otherwise well behaved process.

Smith Predictor Implementation

At this point in the case study, the process transfer function is second order plus dead time while Picles employs a first order plus dead time Smith predictor controller model. This scenario was created to show that although a good model prediction is essential to success, some model mismatch can indeed be tolerated if the model parameters are properly specified.

In the discussion associated with Fig. 7, Digest had computed a Kp of 1.22, a τ_P of 143.1 seconds and a θ of 78.46 seconds from the pulse test of the second order plus dead time transfer function of Eq. 2. Since these model values reasonably describe the dynamic behavior of the transfer function, they are entered into Picles' Smith predictor design menu and the specification of the controller model is complete.

Appropriate PI tuning parameter values must now be determined. Since the Smith predictor controller model compensates for dead time, it seems reasonable that the PI controller should be tuned as if no dead time exists. That is, a $K_{\rm C}$ of 1.529 and a $\tau_{\rm I}$ of 138.4 seconds as used in Fig. 5 should provide similar performance here. Although this logic is reasonable, the mismatch between the first order plus dead time controller model and the second order plus dead time process transfer function means that the approximation of Eq. 3 does not hold true. As a result, if a $K_{\rm C}$ of 1.529 and a $\tau_{\rm I}$ of 138.4 seconds are entered into the Picles controller design menu, the set point step response of the closed loop system is very sluggish, producing no overshoot.

A second idea is to attempt a Ziegler-Nichols closed loop tuning. The procedure for Ziegler-Nichols tuning is to implement a P-Only controller, perturb the process near the desired point of operation and search for the smallest controller gain which effects sustained oscillations in the measured variable. These oscillations should neither grow nor die and the manipulated variable should remain unconstrained. The controller gain at this condition is the ultimate gain and the period of oscillation in the measured variable is the ultimate period. These ultimate values are then used in relations to compute initial controller settings. Unfortunately, a pure P-Only controller does not include the influence of the controller model and thus produces results of no value for model based controller tuning. If the controller model is left in place and a P-Only controller is implemented, the Ziegler-Nichols tuning relations are no longer valid.

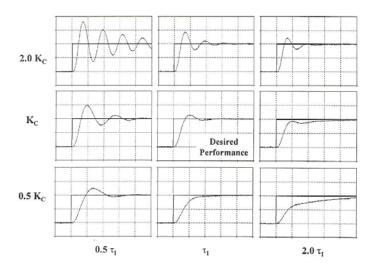


Figure 9 - Tuning map guides trial and error tuning of PI controller

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Consequently, trial and error tuning becomes necessary. Although trial and error is required, tuning can be approached logically. Fig. 9 displays a tuning map which shows how the set point response of a PI controller varies as K_C and τ_I vary. Although this tuning map was generated from a traditional PI controller without Smith predictor, it still provides a useful guide for the trial and error tuning.

The center of Fig. 9 shows a set point step response which is much like the performance desired for this case study. The grid of plots reveal how a set point step response changes as the tuning parameters are doubled and halved from these desired values. The plot in the upper left of the grid shows that when gain is doubled and reset time is halved, the controller produces large, slowly damping oscillations. Conversely, the plot in the lower right of the grid shows that when controller gain is halved and reset time is doubled, the response becomes extremely sluggish.

The very sluggish response which occurs when using a KC of 1.529 and a τ_I of 138.4 seconds is similar to that shown in the lower right of the tuning map of Fig. 9. Hence, to move performance toward the center, the actions opposite of those used to create the lower right tuning map response must be implemented. That is, KC must be doubled (or at least substantially increased) and τ_I must be halved (or at least substantially decreased).

After a few trial and error iterations, Fig. 10 shows the final result. The design criteria of tracking set point steps

from 50% up to 60% with a 10% peak overshoot ratio and complete settling in one cycle of the measured variable is obtained with the tuning of $K_C=5$ and $\tau_I=75$ seconds. As shown, these values achieve settling in about 11 minutes, which compares favorably with the 10 minutes of the no dead time case of Fig. 5. Rise time, at about 3.0 minutes, compares favorably with the 2.5 minutes for the no dead time case.

Homework

The Smith predictor seems to have solved the case of the diabolical dead time - or has it? First, it must be determined how the sensitivity of the controller model parameters, and in particular dead time, impact the performance of the controller. In effect, there are now five adjustable parameters for controller design - three for the FOPDT controller model and two for PI controller tuning.

Other studies might include investigating how the FOPDT dynamic form succeeds as a controller model for a third order plus dead time process or for a process that includes a large lead element. The benefit of a Smith predictor might be investigated when a full PID controller is employed or when the objective is disturbance rejection rather than set point tracking. Use your imagination to develop a variety of process dynamics and control case studies using Picles and Digest.

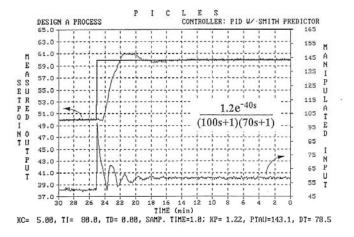


Figure 10 - PI controller with Smith predictor produces the design 10% overshoot, complete settling in 11 minutes and a rise time of 3.0 minutes

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For More Information

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

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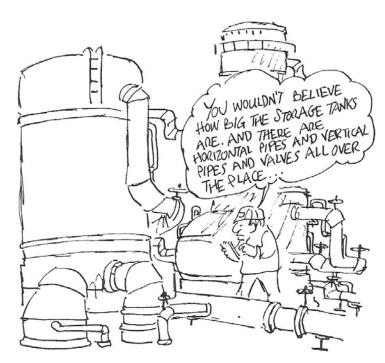
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Literature Cited

- Cooper, D. J., "Picles and the Case of the Interacting Controllers," CACHE News, 40, 3 (1995).
- Cooper, D. J., and J. Bieszczad, "Picles and the Case of the Jacketed Reactor," CACHE News, 39, 24 (1994).
- Cooper, D. J., "Teach Hands on Process Control with Picles," CACHE News, 38, 24 (1994).



Maybe we shouldn't have taken the "K" out of picles!

Dyadem International Ltd. Provides A New Educational Tool

By Michael Seldon, Dyadem International Limited

DDM-HAZOP Professional Version

Students now have the unique opportunity to train on industry standard risk software as used by risk professionals. Dyadem International Ltd. has released a very powerful WindowsTM based Process Hazard Analysis (PHA) tool - DDM-HAZOP. This program has been extremely well received around the world in only a very short period of time. This software makes Process Hazard Analysis easier to perform, less stressful, and much less time consuming.

The Academic Tool

Dyadem International Ltd. is pleased to announce the release of a special software package for all recognized educational institutions.

Since the program has extensive *Help files* and a *detailed tutorial*, students at both the undergraduate and graduate level can now develop a firm understanding of process hazard analyses using a professional risk assessment tool. This state-of-the-art software has extensive Knowledge Based Libraries that reflect high levels of industrial expertise.

This package can be licensed to academic institutions for a fraction of the cost to industrial users.

Major Features of the Program

Major features of the program include:

- HAZOP (including Traditional, Deviation based, Procedural and Plant Modification).
- What If?
- FMEA
- Preliminary Hazard Analysis

The "Naming Convention" and "Item Selection" permit a wide variation of options. This allows the user to customize the program for different methodologies and different formats.

DDM-HAZOP uses a vertical recording format and a horizontal reporting format. Use of the vertical format for recording focuses the team's attention while the horizontal format is best suited for reports. Other attractive features include:

- Extensive and Extendible Knowledge Based Libraries
- · Action Item Management for Post PHA Management
- · Powerful Copying Features for Data Reusability
- High Quality Reports

System Specifications

- · IBM- compatible with 80386 processor or higher
- 3.5 inch floppy disk drive
- · Hard disk with at least 6 MB of free space
- Graphic display device compatible with WindowsTM 3.1 or later. VGA recommended
- · 4 MB of available memory
- Microsoft WindowsTM 3.1 or later (standard or enhanced mode)

About Dyadem International Ltd.

Dyadem International Ltd is a software development organization that specializes in creating risk assessment software for risk professionals. This advanced PHA software is extremely user friendly and highly versatile. Dyadem is associated with a substantial number of companies around the world who supply risk assessment services and also act as DDM Support Members. DDM Support Members teach courses in risk assessment and perform Process Hazard Analyses for a wide range of industries. For more information please see our web page.

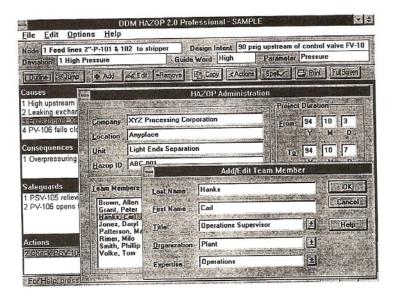
Ordering the Program

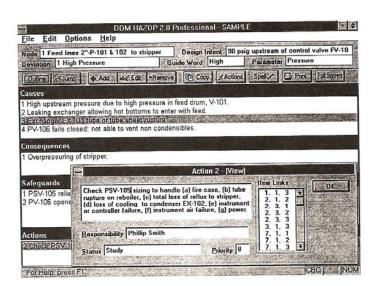
For further information about DDM-HAZOP you may either download a demonstration version from our web page or contact us directly.

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ChemSep Release v3.1

By Ross Taylor and Hendrik A. Kooijman, Clarkson University

History

In 1993 CACHE made available ChemSep Version 2, our program for simulating multicomponent separation processes (Kooijman and Taylor, 1992). Since then more than 40 universities around the world have licensed ChemSep for use in undergraduate, graduate and short courses. Early in 1995 CACHE released Version 3 of the ChemSep package. This article looks at what is new and improved.

The Nonequilibrium Model

The equilibrium stage model has been the standard model for modelling distillation, absorption, stripping, and extraction operations for over a century. The model is based on an assumption that the streams leaving a stage are in equilibrium with each other. The material and energy balances for the whole stage are solved together with equations that represent the assumption of equilibrium in order to obtain product (as well as internal) flow information. The model equations often are referred to as the MESH equations. The equilibrium stage model is so simple in its conception, so elegant from the mathematical viewpoint, has inspired so many algorithms, and has been used to simulate and design so many real columns (and, until now, was the only model in the CACHE release of ChemSep), that it seems impolite to mention that the model is fundamentally wrong! The trays or packings in an actual column are not equilibrium stages.

Separation processes involve the transport of mass and energy between different phases (in columns normally between a vapor and liquid or a liquid and liquid) at rates that depend upon the extent to which the phases are not in equilibrium with each other. The usual way of getting around the assumption of equilibrium is to use an efficiency factor of some kind. If engineers use an efficiency at all, it is most likely to be either the overall efficiency or the Murphree stage efficiency, as they are the easiest to use within the context of the equilibrium stage model.

However, for multicomponent or non-ideal systems both theory and experiment show that efficiencies in multicomponent systems are not the same for all components and, in fact, are functions of the composition, with a range that can vary outside the expected range (zero to unity) from -∞ to +∞ (see Krishna and Taylor, 1993). The assumption of thermal equilibrium (equal temperatures of the streams exiting a stage) can also cause problems. In some operations the phases brought into contact have very different temperatures. To assume that within one stage these phases have exchanged enough energy to equilibrate their temperatures requires either an infinitely large phase interface or an infinitely large heat transfer coefficient. Neither is likely in practice. Worse, there is no easy way of defining an efficiency factor that represents thermal nonequilibrium as may be possible for the chemical equilibrium assumption.

A nonequilibrium model that eliminates the use of efficiencies and models heat transfer was proposed by Krishnamurthy and Taylor (1985) and further developed in a series of papers leading to a second generation model developed by Taylor *et al.* (1994). This is the model implemented in ChemSep Version 3.

In these nonequilibrium models the conservation equations are written for each phase in contrast to the overall stage balances used in the equilibrium model. Mass and energy crosses the interface(s) that separate(s) the phases, driven by the differences between the composition and temperatures in the bulk phase and at the interface (see Figure 1). At the interface itself, the two phases are assumed to be in equilibrium, and the interface compositions and temperature can (and do) differ from those of the two bulk phases. The transport rates are calculated from models of mass transfer in multicomponent systems. Mass and heat transfer coefficients and interfacial areas must be computed from appropriate correlations or from theoretical models. These coefficients depend on the column design as well as its method of operation. It is, therefore, essential to ensure that flows and design parameters are consistent with the satisfactory operation of the column.

Nonequilibrium models can also simulate packed columns simply by using different performance correlations. Though packed columns are continuous contact devices, nonequilibrium stages can be used to model a "short" section of column, representing a discrete integration over the packed bed. Doing so eliminates the need for the Height Equivalent to a Theoretical Plate (HETP), a concept widely used in packed column design but one which suffers from

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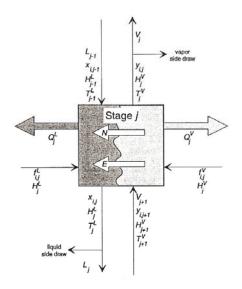


Figure 1. Schematic Diagram of a Nonequilibrium Stage (after Taylor and Krishna, 1993)

the same problems that plague tray efficiencies. A nonequilibrium model can even handle columns with both trays and packings.

Both nonequilibrium and equilibrium models need similar specifications. Feed flows and their thermal condition must be specified for both models, as must the column configuration (number of stages, feed and sidestream locations etc.). Additional specifications that are the same

for both simulation models include the specification of, for example, reflux ratios or bottom product flow rates if the column is equipped with a condenser and/or a reboiler. The specification of the pressure on each stage is necessary if the pressure drop is not computed; if it is, only the top stage pressure needs be specified (the pressure of all other stages being determined from the pressure drop equations that are part of the model described above).

Table 1. Currently Supported Column Internals for the Nonequilibrium Model

Bubble-cap trays
Sieve trays
Valve trays (including double weight valves)
Dumped packings
Structured packings
Equilibrium stage (with Murphree stage efficiency)
Rotating Disk Contactor (RDC) compartment (for extraction)

Spray column stage (for extraction)

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Table 2. Tray Layout Data

General (sieve) tray layo	ut data:		
Column diameter	Active area		
Number of flow passes	Total hole area		
Tray spacing	Downcomer area		
Liquid flow path length	Weir length		
Hole diameter	Weir height		
Hole pitch	Deck thickness		
Downcomer clearance			
Additional data for bubble caps:			
Cap diameter	Slot area		
Slot height	Riser area		
Skirt clearance	Annual area		
Additional data for valve	es:		
Closed Loss K	Open Loss K		
Eddy Loss C	Ratio Valve Legs		
Valve Density	Valve Thickness		
Fraction Heavy Valves	Heavy Valve Thickness		

The nonequilibrium model, in comparison with the equilibrium model, requires the evaluation of many more physical properties and of the heat and mass transfer coefficients. In addition, a nonequilibrium simulation cannot proceed without some knowledge of the column type and the internals layout. Tray type and mechanical layout data, for example, is needed in order to calculate the mass transfer coefficients for each tray. For packed columns the packing type, size and material must be known. Libraries with standard tray and packing data are available on-line. Table 1 lists the currently supported types of column internals.

Tray layout parameters that complete a column design (needed for the calculation of mass transfer coefficients and pressure drops) are shown in Table 2. For packings only the column diameter and bed height are design parameters, other parameters are fixed upon the selection of the type of packing (such as void fraction, nominal packing diameter, etc.). The packed bed height must be specified since it determines the desired separation and the capacity.

If no column layout data is available, the program has an optional design mode that automatically assigns internal equipment parameters. The user just needs to select one of the types of internals (for each section in the column). The design-mode is activated by not specifying the column diameter (leaving it as a "default" with "*") for a specific section. With the design-mode "on" the design for each tray is automatically adapted during an iteration and the layout is rationalized for each specified section in the column.

One of two different design methods can be employed:

- Fraction of flooding; this is the standard design method for trays.
- Pressure drop; this is the usual design method for packed columns, but is very useful as well for tray design with pressure drop constraints.

The methods generate a column-design that might not be optimal from an engineers viewpoint but can be considered to be sensible starting points for an actual design.

Example: Extractive Distillation

This example is problem 7-F2 from King (1980), where we want to separate an equimolar mixture of methylcyclohexane (MCH) and toluene, and do this by extractive distillation with phenol as the solvent. The flowsheet is shown in Figure 2, where we set the total feed flow rate is 20 mol/s (as the nonequilibrium model works with actual tray performances actual feed flow rates are required). Since the column efficiencies are less than unity more actual trays are required than the number of equilibrium stages specified by King. Here 38 valve trays are used and the nonequilibrium model in design mode to generate the tray layout. A total condenser and partial reboiler are used (stages 1 and 40), the phenol recycle (at 100°C) enters the column on the 5th tray, and the fresh-feed enters on the 26th tray (at it's bubble

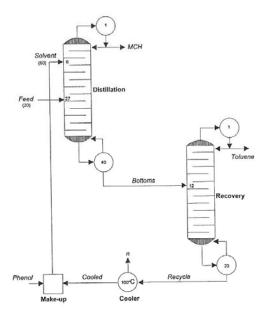


Figure 2. Extractive Distillation of Methylcyclohexane and Toluene with Phenol as Solvent

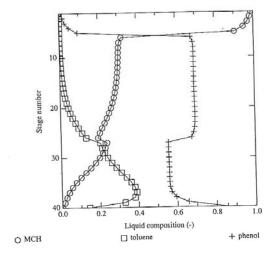


Figure 3. Liquid MoleFraction Profiles for the Extractive Distillation of Methylcyclohexane and Toluene with Phenol as Solvent.

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point). The DECHEMA — UNIFAC model is used for the thermodynamics (default physical property models are used). The liquid composition profiles obtained by ChemSep are shown in Figure 3.

The phenol raises the relative volatility of methylcyclohexane with respect to toluene so that a methylcylcohexane product is taken as overhead and the toluene leaves the bottoms together with the phenol. For a high purity product the solvent feed to fresh-feed ratio as well as the reflux ratio needs to be sufficiently high. However, using too much phenol will increase the cost of the operation unnecessarily. The column design mode has sized the column in three different sections with diameters of 1.7 m, 1.65 m and 1.77 m respectively. The main difference in tray layouts is a smaller downcomer area in the top section, as the (cold) phenol feed introduces a lot of liquid in the column, which mainly goes down the column.

In Figure 4 the back-calculated Muphree component efficiencies are plotted for the three components. The efficiency of phenol varies considerably and also the efficiencies of methylcyclohexane and toluene change in the bottom of the column.

Figure 5 shows the pseudo McCabe-Thiele diagram for the pseudo-binary MCH and toluene. Even though the pseudo McCabe-Thiele plots sometimes look rather strange (for example, here the equilibrium line jumps a bit around the feed tray) they can be quite useful for the analysis and feed tray selection in multicomponent separations.

The bottoms stream containing the toluene and phenol is sent to another distillation column where the phenol is recovered and toluene is produced. After simulating the extractive distillation column, the phenol recovery column, and the recycle cooler, we can now combine the various sepfiles into one flowsheet. To solve this flowsheet by hand is tedious and requires a lot of manual labor. In the new release (v3.1) of ChemSep a new program, called FS, can solve the whole flowsheet by calling ChemSep programs sequentially. The extractive distillation process, as well as other processes such as the azeotropic distillation of benzene and cyclohexane with acetone, the binary heterogeneous azeotropic distillation of n-butanol and water, and a liquid-liquid extraction with solvent recovery are provided as worked examples.

Other improvements

While the inclusion of the nonequilibrium model is the most significant addition to the ChemSep package, there are many other improvements and new features including:

 A new program, called ChemProp, has been added to the package. ChemProp can compute physical properties such as densities, viscosities, etc.

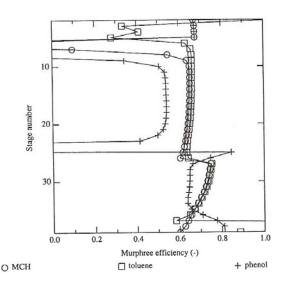


Figure 4. Component Murphree Efficiencies for the Extractive Distillation of Methylcyclohexane and Toluene

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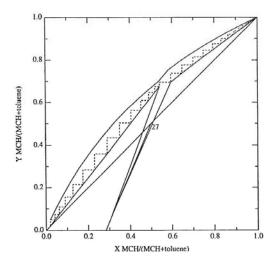


Figure 5. McCabe-Thiele Diagram for the Extractive Distillation of Methylcyclohexane and Toluene with Phenol as Solvent

- On line technical manual, available with F9. Also available in PostScript format from our FTP-site (see below). It contains detailed information on the models that are implemented in ChemSep.
- Flexible specifications for the condenser and reboiler.
 This means you can provide a specification like MB = 20 [kg/s], meaning that the mass flowrate of the bottom product is 20 kg/s. Any stage variable or stream molecular weight may be specified. This also means that it is now possible to specify both the reflux ratio and distillate flow rates. In prior releases it was necessary to specify the reflux ratio and bottoms flow rate.
- Instant unit conversions: F11 allows the conversion of any two compatible units.
- Improved plots. You can now import or export specific profiles and the component selection of McCabe-Thiele plots now also handles azeotropic and extractive distillations correctly. You can select the font type, font size, and line width for PostScript plots.
- A new file viewer can read files of unlimited size and has a search engine (Ctrl-S/Ctrl-N). It is used to view the technical manual online.

- Virtual memory support allows the simulation of big problems with little extended memory available (maximum 200 stages and 10 components).
- Searching components by property values is improved by allowing the specification of the property units.
- A new automatic initialization method improves the convergence for purity or recovery specifications.

The latest news on ChemSep may be found on our World-Wide-Web (WWW) page, http://fire.camp.clarkson.edu/~kooijman/ and you can download files not on the distribution disks from our FTP-site, rt.che.clarkson.edu (128.153.18.116), login: chemsep, password: cs21. The WWW-pages are still under development. We would like to provide FTP-service also through the WWW-pages at a later date.

Acknowledgements

Support for our research and the development of nonequilibrium models is provided by BP International and Hyprotech limited. We are also collaborating with Professor A. Gorak and his group at the University of Dortmund.

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References

R. Taylor, H.A. Kooijman, J-S. Hung, "A Second Generation Nonequilibrium Model for Computer Simulation of Multicomponent Separation Processes", *Comp. Chem. Eng.*, Vol. 18, No. 3, (1994) pp. 205-217.

R. Taylor, R. Krishna, Multicomponent Mass Transfer, Wiley, New York (1993).

J.C. King, Separation Processes, 2nd Edition, McGraw-Hill, New York (1980).

H.A. Kooijman, R. Taylor, "ChemSep - Another Software System for the simulation of Separation Processes", *CACHE News*, Fall 1992, No. 35, pp. 1-9.

For More Information

To obtain more information on Chemsep v 3.1, please contact:



POLYMATH Numerical Computation Package New Release - Version 4.0

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

The POLYMATH package has undergone significant improvements during the last year, and the latest version is now available from CACHE. New features and capabilities include:

Simultaneous Differential Equation Solver

The number of equations has been increased to 31 with three lines now allowed per equation. The default integration algorithm is now the Runge-Kutta-Fehlberg 4th-5th order with relative error of 10^{-10} and no limit on step size. A selectable stiff algorithm uses the Bader-Deuflhard semi-implicit extrapolation method. A new storage algorithm uses the available conventional and extended memory (XMS) to store data at each integration step for accurate plotting, and data compression is only used as necessary. Graphs may be scaled and labels added before printing.

Simultaneous Algebraic Equation Solver

The number of equations has been increased to 32 with three lines now allowed per equation. An improved bounded Newton-Raphson method is used which eliminates intervals where functions are undefined from the solution. The program will now calculate and display the auxiliary equation solutions even if there are no nonlinear equations to solve.

Simultaneous Differential Equation Solver and Simultaneous Algebraic Equation Solver

Logical expressions with the if (condition) then (expression) else (expression) syntax are now allowed. The condition may include the following operators: >, <, >=, <=, == (equals), >< (does not equal), | (or) and & (and). The expressions may be any formula, including another "if" statement.

Polynomial, Multiple Linear and Nonlinear Regression

The residual plots for all types of regression can now be automatically determined and plotted, and the calculated regression results are now available to the working data table.

Linear Equation Solver

The linear equation solver is now a separate program which can solve up to 32 equations. Input to a spreadsheet-like form is accomplished with keyboard entry via the arrow keys or can be read from a DOS file. Algebraic expressions with all intrinsic function are accepted as input.

All Programs

The following functions are now available in all programs as well as the calculator:

In (base e) abs (absolute value) arcsin sinh log (base 10) int (integer part) arccos cosh exp (e^x) frac (fractional part) tan arctan tanh exp2(2^x) round (rounds value) arcsec arcsinh exp10 (10^x) sign (+1/0/-1) csc arccsc arccosh sqrt (square root) cbrt (cube root)

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arccot

arctanh

New printers and graphics files are supported. Equations and data are now printed as text rather than graphics to improve clarity.

Verification is now requested before changes to the current problem can be lost (by loading a different problem or leaving the current problem).

The copying of problems between libraries is now facilitated.

POLYMATH Trial Offer

You may request this package from CACHE for testing and evaluation. If you decide to obtain POLYMATH for possible classroom or department use, please note the conditions indicated in the order form given below:

POLYMATH Order Form

Educational licenses: If you decide to obtain POLYMATH for testing (see form below), please be aware of the following:

- 1. You may reproduce the program as many times as you like for students and other faculty.
- 2. Your department chairman will be informed of the testing.
- If you decide to use POLYMATH in your department after 3 months, your department will be billed for \$125, and \$75 for
 each successive year thereafter. This fee covers any updates or new versions. Nonmember institution rates are an
 initial \$150 and a \$100 annual fee.
- 4. If you decide not to use POLYMATH after 3 months, you must return (or certify you have erased) all copies made.

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

Individual student copies are \$25 each.

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CACHE CD-ROM (Volume 2)

By Peter R. Rony, Virginia Tech and Michael B. Cutlip, University of Connecticut

Background for Volume 2

CACHE Corporation celebrated its 25th anniversary last year at the AIChE Annual Meeting in San Francisco (November 1994). One of its anniversary activities was the creation and distribution of 2000 copies of a 25-anniversary CACHE CD-ROM for chemical engineering students and faculty. This CD-ROM contained 678.2 megabytes of educational and demonstration software of interest to chemical engineers. The success and attention associated with the 25th Anniversary CACHE CD-ROM catalyzed interest in making the CD-ROM production and distribution an annual event.

The Volume 2 CACHE CD-ROM will be replicated for initial distribution at the AIChE Annual Meeting in Miami Beach starting November 12, 1995. As with the first CACHE CD-ROM, students who attend the AIChE Student Brunch on Sunday (10-11 a.m. Grand Ballroom, Versailles Building) will each receive a free copy, as will faculty who attend the CACHE Reception on Wednesday evening. Individual CD-ROMs will then be made available to students, faculty and departments — at a price to be determined by production and royalty costs — from the CACHE office in Austin.

As the use of CD-ROM drives becomes pervasive, this method of software distribution has the potential to reach most chemical engineering students each year with updated and new educational materials.

Late in 1995 we hope to produce and distribute at least 2500 Volume 2 CD-ROMs. The objectives of the Volume 2 CACHE CD-ROM were the same as they were for Volume 1: (a) to demonstrate new computer technology useful in chemical engineering education, and (b) to provide a set of software deliverables to the target audience — ChE students and faculty — for the CD-ROM.

Software contributions from industry and academia were solicited, starting in June 1995, by CACHE for the Volume 2 CD-ROM. Contributed software was required to have a strong educational value or impact, to be of general interest to chemical engineering students and faculty, and to execute properly. It was noted that students and faculty prefer to have software run directly from the CD-ROM so that they do not tie up much of their valuable hard disk

storage. CACHE reserved the right to refuse submitted materials because of subject, quality or storage requirements.

What software is of interest to CACHE for its CD-ROM series, not only for Volume 2 but for succeeding volumes throughout the 1990s? As an example, software contained on the Volume 2 CACHE CD-ROM disc can be subdivided into the following categories:

Category I. Modern Programming

Students in the future will more likely use programming tools based upon object-oriented programming, reusable components, visual development tools, and so forth. Examples are Borland s Delphi and Microsoft s Visual Basic and Visual C++.

Category II. Modern Application Programs

A wide range of applications that apply, in principle and in practice, to chemical engineering, including data analysis, scientific visualization, chemical process simulation, process design, process control, spreadsheets, 3D modeling virtual reality, and so forth.

Category III. Modern Communication of Information

Students in the future will more likely use a variety of software to communicate concepts, results, and conclusions via a variety of data types — text, images, audio, animation, and video. Category includes written, oral, poster, and Internet communications.

Category IV. ChE Departmental Information

This category will provide all departments with the opportunity to communicate information on their particular department, specially major activities that would be of interest to potential students. Such material can include undergraduate or graduate (electronic) brochures on the department, or information on particular research centers. High-quality, general material on chemical engineering are also welcome. The use of HTML scripts and GIF files—associated with World Wide Web—is particularly welcome.

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Category V. Information from Chemical Engineering Faculty and Authors

This category will be available to individuals who would like to provide information to ChE students and faculty. Authors can provide additional materials to supplement their textbooks or their software, overheads of pertinent chemical engineering theory, and so forth. New ideas for visual or audio ChE information communication can be tested.

Category VI. Information Sources for Chemical Engineers

The material in this category will include sources for chemical engineering information and literature. Examples here can include listings of chemical engineering textbooks by various publishing houses along with the outlines of the individual textbooks and perhaps even a sample chapter, complete with figures and tables. Commercial databases of information relevant to chemical engineering also can provide information and sample database use to ChE students and faculty.

Submission Suggestions for Volume 2

A variety of software can be used to communicate information and materials. Examples of such software are linear presentations (e.g., Lotus Freelance, Microsoft Power Point), Hypertext (including Adobe Acrobat with links), multimedia presentations (e.g., Authorware, Director, Multimedia Toolbook), specialized demo software (e.g., Lifeboat's Demo-It!), or sub directories of HTML scripts, GIF files, etc. that can be viewed with a local WWW Windows-based viewer on the CD-ROM disc such as Null Mosaic. Any output that can be placed in Postscript (PS) or encapsulated Postscript (EPS) can be converted to a PDF file by the editor and viewed by Adobe Acrobat Reader for Windows/Mac software on the CD-ROM.

Contributions were requested primarily for either the Windows or Macintosh platforms, although DOS contributions were also solicited. Contributed materials should be thoroughly tested prior to submission (serious problems with execution led to the exclusion of an occasional program). No overall, organizing GUI will be provided for Macintosh files (the Mac folders adequately organized such information). World Wide Web HTML and GIF files were submitted since a local WWW browser — null Mosaic or Netscape — located on the CD-ROM was available to users to view these files. In fact, the local WWW presentation could take advantage of audio, video on the CD-ROM disc.

Contributors of DOS software were asked to be aware of the following pitfalls:

 Some DOS programs incorporate self-modifying code and cannot be executed from a ROM such as a CD-

- ROM disc. These DOS programs must first be installed on the hard drive from the CD-ROM.
- 2) Some DOS programs cannot be executed from a DOS window within Windows 3.1x. One must leave Windows in order to execute such programs, which are a great nuisance and sidestep the advantages of CD-ROM technology. The editors reserve the right to omit these specific DOS programs from Volume 2 if there are severe space limitations.

Submission Timing

Contributors were requested to submit fully tested CD-ROM materials by September 1, 1995, or sooner. Floppy disks were the preferred medium of submission; however, the use of Internet FTP was an acceptable method for the transfer of large files that did not fit on a floppy diskette. With FTP submission it was recommended that the contributor follow up with the editor to make certain that he accessed, received, and tested the FTP-transferred file.

Costs associated with Submissions

CACHE is providing this CD-ROM and its contents as an education service to chemical engineering students and faculty. There were no charges to contributors of the Volume 2 CACHE CD-ROM; however, unrestricted financial contributions from companies, corporate foundations, and other sources were solicited and greatly appreciated to help offset the costs of the CD-ROM preparation, reproduction, and distribution.

Material From Volume Will appear in Volume 2

The available supply of Volume 1 (25th-Anniversary) CACHE CD-ROM discs from CACHE headquarters in Austin, Texas was exhausted by May, 1995. Rather than replicate an additional batch of 500 - 1000 discs, it was decided to create a Volume 2 CACHE CD-ROM based upon the Volume 1 CD-ROM disc files plus supplementary files obtained through the June 1995 solicitation. Space for new material would be made available by the deletion of the 214-megabyte Mobil Oil video file (MOBIL. AVI), originally present on the Volume 1 disc, as well as by the deletion of files that produced execution problems. The available space for new files - e.g., ChE departmental presentations, scientific visualization examples, Delphi examples, and so forth - on the Volume 2 disc will be approximately 250 megabytes - as much as 36% of the CD-ROM disc. For the editor, it was nether feasible nor appropriate to produce a 100% new CACHE CD-ROM during the summer of 1995.

In Summary

All chemical engineering departments and faculty—as well as major corporations that provide modern programming, application, and communication software—were invited to participate in the adventure of Volume 2. Volume 2 and future volumes of the CACHE CD-ROM will remain as a testbed for new ideas in the application of software in chemical engineering education.

CACHE CD-Rom - Volume 2 Order Form			
The CACHE CD-ROM - Volume 2 is now available for sale from the CACHE office. Details of the attached. Supporting academic departments and all AIChE Student Chapters may order individual C supporting departments may order the CD at \$10 each. Individual CD's will be \$10 for students at others. The supply is limited so orders should be placed as soon as possible.	D's at \$5 per copy. Non-		
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ANNOUNCEMENTS

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January 7-12, 1996

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James Rawlings	University of Wisconsin (USA)
Sigurd Skogestad	University of Trondheim (N)

ABOUT THE CONFERENCE

Chemical Process Control - V (CPC-V) will bring together engineers and scientists from universities, the processing industries, government laboratories to assess and critique the current and future directions of research in chemical process control. CPC-V is the fifth in a series of international conferences held every five years commencing in 1976.

The goals of CPC-V are to:

- promote a vital, interactive discussion among a diverse group of experts regarding the state of the technology for chemical process control,
- assess current research,
- identify research opportunities for academics, government, and industry, and
- (4) promote productive research collaborations.

Conference participants will have ample opportunity to interact with peers and experts in their fields.

CONFERENCE FORMAT

The conference will be organized into morning and evening technical sessions that address current issues in process control. The sessions will consist of two or three papers followed by a formal critique or discussion. There will be at least an hour in each session reserved for audience participation in the discussion. The afternoons will be free for further informal discussion. A session for contributed poster papers is also planned.

To achieve the conference goal of interactivity, there will be many opportunities discussion and social interaction. Meals will be taken together in the morning and evening. Breakout rooms will be available for afternoon discussion. There will be daily refreshments, an opening reception, and a Thursday night conference banquet.

CONFERENCE THEMES

The main themes of the conference include:

Surveys and Assessments of current research areas

- Robust & predictive control
- · Modeling and identification
- · Nonlinear & Adaptive control

New research directions

- · Process monitoring and fault detection
- Sequence control, PLC's, and discrete event systems

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· Sensors and data fusion

Surveys of control practice in industry

- Food processing
- · Refining and chemicals
- Pulp & paper
- The nontraditional process industries

Status of Industry/Academic Research

Twenty years have passed since CPC-I. What has been accomplished, and what are the prospects?

- What have been the directions and results of government and industry sponsored research.
- When does joint academic/industry research pay off?
- What are the prospects?

LOCATION

The Granlibakken Conference Center is near Tahoe City, California, located on the north side of Lake Tahoe in high Sierra Nevada mountains. It is a one hour drive from the Reno Cannon International Airport in Reno, Nevada. The Reno airport is served by America West, American, Continental, Delta, Reno Air, Southwest, Sky West, United, and U.S. Air. There is a van service between the Reno airport and the Conference Center.

Winter recreational activities are available at the conference site and at nearby major ski resorts. The conference center offers a small ski facility with surface lift, ski rental shop, ski school, and cross-country ski trails. A free shuttle takes you to the Squaw Valley and Alpine Meadows ski areas. Restaurants and fine shops are nearby. There is bus and boat service to the major tourist and entertainment areas located in South Lake Tahoe.

CONFERENCE SCHEDULE

The conference features nine technical sessions held in the mornings and evenings. Except on Thursday, afternoons will be free for informal discussions, demonstrations, or recreation. A Thursday afternoon poster session will be followed by an evening banquet.

The conference will begin with an evening session following dinner on Sunday, January 7, and conclude following lunch on Friday, January 12.

CONFERENCE PROGRAM

Session 1: Opening Session (Sunday, January 7, 7:00 - 9:30 pm)

Chair: Carlos Garcia (Shell Chemical Company)

Objectives and Agenda for CPC-V Carlos Garcia (Shell Chemical Company) and Jeffrey Kantor (University of Notre Dame)

Assessment of Process Control in the Petrochemical Industries

George Birchfield (Solomon)

The Future of Advanced Control
Brian Ramaker, Henry Lau, and Evelio Hernandez (Shell
Development)

Session 2: Adaptive and Nonlinear Control — Fact or Fantasy? (Monday, January 8, 7:45 - 11:30 am)

Chair: Yaman Arkun (Georgia Institute of Technology)

Certainty Equivalence Adaptive Control: Paradigms, Puzzles and Switching

B. Erik Ydstie (Carnegie Mellon University)

Nonlinear Process Control — Which way to the promised land?

Frank Doyle (Purdue University) and Frank Allgower (Universitat Stuttgart)

Industrial Applications of Nonlinear Control
Babatunde Ogunnaike (Dupont) and Raymond Wright (Dow
Chemical)

Session 3: Industrial Survey — II (Monday, January 8, 7:30 - 10:00 pm)

Computer Aided Process Engineering in the Snack Food Industry

Mike Nikolau (Texas A&M University) and Don Strickert (Frito-Lay Technology)

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Batch Food Processing: The proof is in the eating Sandro Machietto (Imperial College)

Session 4: New Directions for Academic Research (Tuesday, January 9, 7:45 - 11:30 am) Chair: Frank Doyle (Purdue University)

Monitoring and Diagnosis of Automated Controllers in the Chemical Process Industries Derrick J. Kozub (Shell Development)

Process Analytical Chemical Engineering Bruce Kowalski (University of Washington)

Analysis and Control of Combined Discrete/Continuous Systems: Progress and Challenges in the Chemical Process Industries

Paul I. Barton and Taeshin Park (MIT)

Session 5: Industry Survey III (Tuesday, January 9, 7:30 - 10:00 pm)

Dale Seborg (University of California, Santa Barbara)

Modeling and Control in Pulp and Paper Industries Ferhan Kayihan (Weyerhaeuser Company)

Case Studies in Equipment Modeling and Control in the Microelectronics Industry

Stephanie W. Butler (Texas Instruments) and Thomas F. Edgar (University of Texas)

Session 6: Impact of Computer Science (Wednesday, January 10, 8:15 - 12 noon)

Chair: Larry Biegler (Carnegie-Mellon University)

Numerical Analysis and Process Control Steven Wright (Argonne National Laboratory)

Real-time Economic Optimization (RTO) of Continuous Plant Operating Conditions

Thomas E. Marlin and Andrew Hrymak (McMaster University)

DES for Processes

Sebastian Engell and Stefan Kowalewski (University of Dortmund) and Bruce Krogh (Carnegie Mellon University)

Session 7: Past and Future Directions of Process Control Research (Wednesday, January 10, 7:30 - 10:00 pm) Chair: John Perkins (Imperial College)

Title TBA
Manfred Morari (ETH-Zurich and Caltech)

The Future of Process Control - a UK Perspective
Roger Benson (ICI and UK Ministry for Trade and Industry)
and John Perkins (Imperial College)

Session 8: Predictive Control (Thursday, January 11, 7:45 - 11:30 am)

Chair: James B. Rawlings (University of Wisconsin)

A Review of Recent Progress in Model Predictive Control Jay H. Lee (Auburn University)

Optimization in Model Based Control
David Q. Mayne (University of California, Davis)

An Overview of Industrial Model Predictive Control Technology

Joe Qin (University of Texas) and Thomas Badgwell (Rice University)

Panel Discussion

Evelio Hernandez (Shell Development Company), Jay H. Lee (Auburn University), David Q. Mayne (University of California, Davis), Joe Qin (University of Texas), and Thomas Badgwell (Rice University)

Session 9: Contributed Poster Session (Thursday, January 11, 1:30 - 3:30 pm)

Chairs: Richard Braatz (University of Illinois) and Karlene Kasonovich (University of South Carolina)

Contributions are invited which address the goals of this conference (no presentation of incremental results!)

Announcements

PARTICIPANTS / CONFERENCE SIZE

The conference will be limited to 150 participants. Prior experience has shown this to be the largest size that can reach the conference goals of cohesiveness and interactivity. The selection of participants will be based on applications; the criteria include diversity by employment (industry, academics, government), residence (US, Europe, Pacific Rim, emerging economies), and experience (graduate students, practitioners, and world class experts).

CONTRIBUTED PAPERS

A poster session is planned to accommodate contributed papers. Submission details will be provided to invited participants.

ACCOMMODATIONS AND MEALS

The Conference Center includes reasonably priced lodging in shared one, two, and three bedroom townhouses with kitchens. All units have TV and direct dial telephones; all bedrooms have private baths. Accommodations will be on the American plan with three full meals.

A variety of lodging packages will be offered, with a basic package to include all meals and double occupancy sleeping accommodations for \$650. There will be moderate additional charges for single rooms, or for an accompanying spouse or guest sharing a room. Participants may wish to extend their stay and enjoy the scenic location and winter regeation.

Further details on room and board packages will be provided later to invited participants.

Instructional Slides for Problem Solving Book

By H. Scott Fogler, University of Michigan and Steven LeBlanc, University of Toledo

The book "Strategies for Creative Problem Solving" by H. Scott Fogler and Steven LeBlanc has a set of 150 color slides of teaching material available for use in the classroom. If you are using this book in one of your courses, you may wish to consider obtaining a copy of the slides. The slides are in Microsoft PowerPoint format and are distributed on disk by the CACHE Corporation. The PowerPoint Viewer is included with the materials, so you do not have to own your own copy of PowerPoint to display the slides. The disks are being made available at a cost of \$15 for the set. Try this new way to "spice" up your classroom presentations and excite your students with some full-color teaching slides.

For more information contact:

Steven LeBlanc Chemical Engineering Department The University of Toledo

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