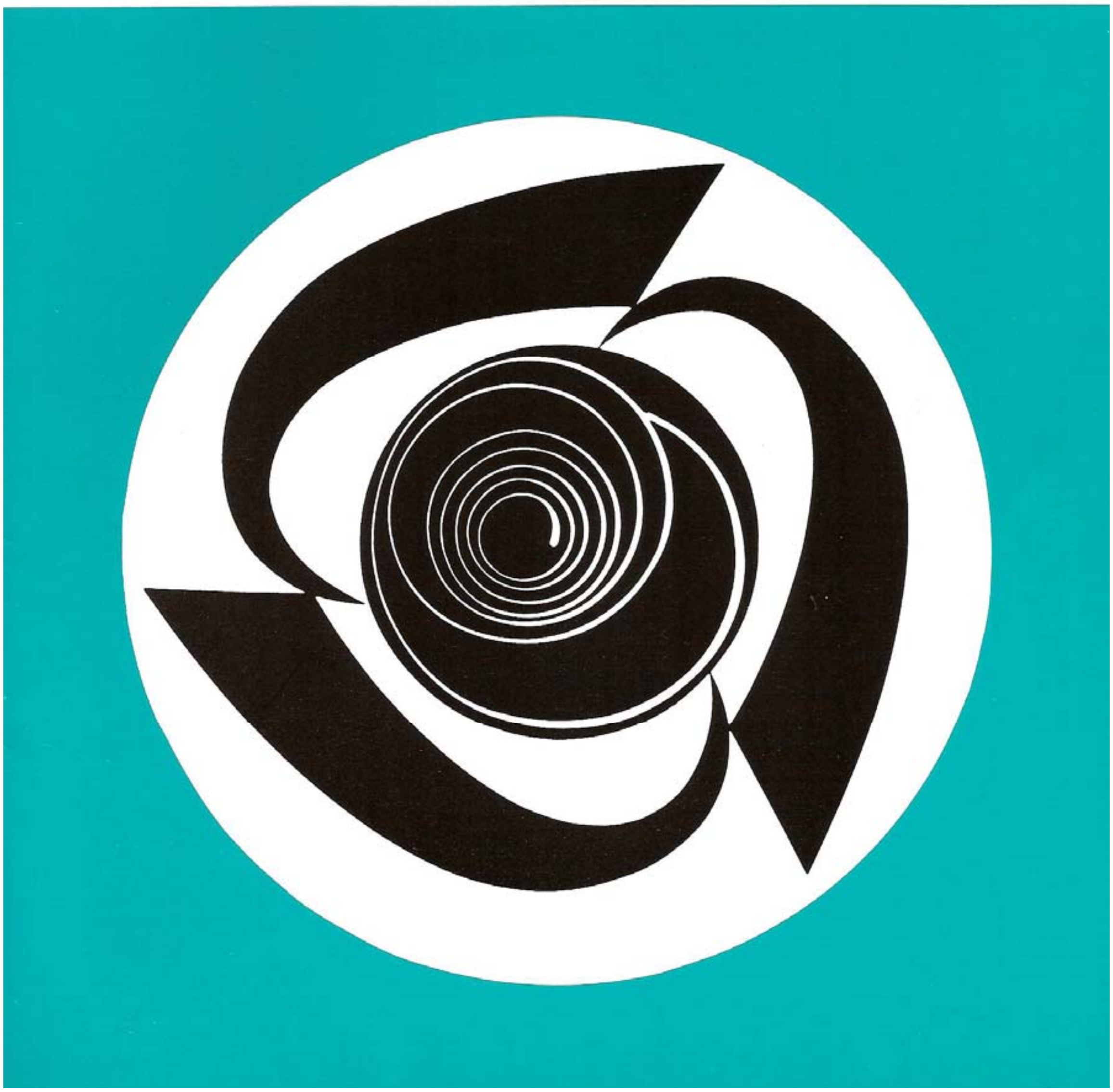
CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 42 Spring 1996



The CACHE CORPORATION

WHAT IS CACHE?

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

CREATION OF THE CACHE CORPORATION

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

CACHE ACTIVITIES

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

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

http://www.cache.org

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.

CACHE NEWS

No. 42 Spring 1996

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CACHE Task Forces and Committees

CACHE CD-ROM (Volume 2)

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

If everything goes according to plan, the Volume 2 CACHE CD-ROM will be distributed to chemical engineering undergraduate students, to faculty, and to CACHE-supporting ChE departments sometime during March or early April 1996. The distribution of Volume 2 was delayed from its initial target date of Sunday, November 12, 1995 at the AIChE Annual Meeting in Miami Beach, Florida. Version VOL2_19 was demonstrated at the AIChE Student Chapter Brunch, Monday, November 12, 1995; during the Educational Software Session 264 all day Tuesday and Wednesday; and the CACHE Reception on Wednesday, November 15, 1995 in Miami Beach. License agreements for free copies of Volume 2 were signed by approximately 500 students, as well as by 200 faculty members and guests at the reception. CD-ROM discs will be sent in one mailing to a ChE department — one copy for the department head/chairman, one copy for the AIChE student chapter, copies for those students who signed up at the AIChE student brunch, and several copies of the Microsoft Development Network Development Library (April 1995 version), a most generous gift to the chemical engineering community courtesy of Dr. Joel P. Kantor, Academic Programs Manager at Microsoft Corporation in Redmond, WA.

The entire December-January holiday period of one month was required both to finish the Authorware 3.01 for Windows graphical user interface (GUI) and to make final decisions on the file content of the 650.8 maximum capacity CD-ROM disc. Beta testing of the VOL2_29 write-once CD-R disc was performed during the end of January and all of February, 1996. The master CD-R disc was completed and sent, for replication of 2500 CD-ROM discs, to 3M Corporation in Menomonie, Wisconsin by the third week of March, 1996. A normal production cycle requires 15 days.

Mike Cutlip was the main beta tester for the series of test CD-Rs that the editor, Peter Rony, produced starting in October 1995. Mike Cheung tested VOL2_29 for use with the Windows 95 platform; he observed that DOS files (examples: XCOPY.EXE and PKUNXIP.EXE) associated with Windows 3.1 gave problems when an attempt was made to execute them on Win95. A critical decision was made to provide only a Windows-based CD-ROM disc. The dual platform approach, with the Macintosh as the second platform, was dropped because HFS filename overhead for the Macintosh-formatted dual platform CD-ROM was about 45 Mb. Little useful material for the CD-ROM was lost by excluding the Mac.

3M Corporation provided the first 1500 CD-ROM discs and disc mastering/artwork charges as a corporate contribution to both CACHE and to the academic chemical engineering community. Several companies, including Laboratory Technologies, Inc. (Fred Putnam, a ChE, is president) have also provided financial support for CD-ROM disc replication and distribution.

What is new on the CD-ROM? Critical installation software is being developed to easily allow installation and operation from any designated CD-ROM drive letter. The Authorware GUI will be based upon Authorware 3.01 rather than 2.01, making navigation easier for the entire graphical user interface. The Authorware 3.01 GUI contains eleven (11) main menu categories:

File
Install
Readme
CACHE
3M
Depts
Demos
HTML
PDF
SciViz
WWW

that provide "perpetual menu" access to most of the contents of the CD-ROM.

There are approximately 678+ million bytes of files on the Volume 2 CACHE CD-ROM. Licenses for a local HTML viewer, called IVIEW version 1.15, and for a Windows-based installation program, Freeman Constructor, have been obtained for all 2500 discs. The use of Freeman Constructor has led to the creation of an CDSETUP.EXE file to install the CD-ROM Authorware graphical user interface for the first time.

What else is new on the CD-ROM? A student version of the DIPPR student database, including instructions. AIChE materials from the New York office regarding student chapters and membership information. Courtesy of Professor Dale Kirmse of the University of Florida and the AIChE Web site at that university; AIChE information on the World Wide Web, including full details of the recent Miami Beach AIChE meeting; these WWW files are viewable using IVIEW or local capabilities of Netscape or Mosaic. WWW publisher information from Prentice-Hall (other publishers were contacted, but did not contribute). Updated demos from Aspen and Sim Sci (other design companies were interested, but were not able to contribute materials this year). Tutorial information on Spyglass' scientific visualization software, including both Slicer (3-dimensional plots) and Transform (2-dimensional plots). Bruce Finlayson's materials on his Chemical Reactor Design Toolbox. The entire CACHE 25th-Anniversary Monograph, except perhaps one chapter, in Acrobat PDF format. Many additional new demo software items. Extensive coverage of shareware and freeware WWW software.

Finally, as an extra feature — call it a bonus — an extensive SETUP.EXE file is provided that allows a CD-ROM user to create several hundred Program Manager icons located within about 10-15 different Program Manager groups.

Pricing for the CD-ROM disc is as follows: $15 each for student chapters and supporting ChE departments. $20 each for non-supporting departments, individual students and faculty. $50 each for ChE professionals who have no academic connection as faculty members. Departments and students who submitted orders based upon incorrect prices contained on page 24 of the Fall 1995 CACHE News will have those prices honored by the CACHE Corporation as a matter of corporate integrity.

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 contents of this CD are attached. Supporting academic departments and all AIChE Student Chapters may order individual CD's at $15 per copy. Non-supporting departments may order the CD at $20 each. Individual CD's will be $20 for students and academics and $50 for others. The supply is limited so orders should be placed as soon as possible.

AIChE Student Chapters may choose to sell the CD-ROM at the $15 cost, or they can charge undergraduate students, graduate students, and faculty up to $20 per CD in order to generate some funds for the Student Chapter.

# OF COPIES		TOTAL
________	$15 each for student chapters and supporting departments	________
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The Picles Training Simulator and The Case of the Fickle Feed Forward

By Douglas Cooper, University of Connecticut

Introduction

Practice in applying textbook theory can greatly benefit the learning process. Such practice is motivating, promotes critical thinking, facilitates understanding of the use and limitations of the theory, and helps prepare students for the challenges of the professional world. For process dynamics and control, Picles^{TM}, the Process Identification and Control Loop Explorer System, is a cost effective way to provide this practice.

Picles is IBM PC compatible software now being used in process dynamics and control courses around the world for the education of students and training of practitioners. Picles is easy-to-use, visually appealing and provides the capability to explore a wide range of process dynamics and control concepts. Thus, students can quickly and inexpensively gain experience which benefits their education.

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

The processes and controllers available in Picles enable the exploration and study of increasingly challenging concepts in an orderly fashion. Early concepts to explore include the basics of process dynamic behavior such as process gain, time constant and dead time. Intermediate concepts include the tuning and performance capabilities of all modes of the PID controller. Advanced concepts include cascade, decoupling, feed forward, dead time compensation and digital control.

After a brief review of program features, this article explores one case study possible with Picles. In this case study, Picles' Heat Exchanger process and Gravity Drained Tanks process are used to explore the design and implementation of a feed forward controller with feedback trim. Based upon these investigations, some design criteria for obtaining benefit from feed forward control are established. As part of the discussion, Digest's dynamic modeling and controller design capabilities are demonstrated.

The Picles Case Studies

Previous *CACHE News* articles describe the Picles processes and present additional case studies [1-4]. 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 implemented and custom tuned in only a few key strokes. The PID controllers can be implemented in any combination of P-Only through full PID. The digital controller permits study of discrete time algorithms such as the deadbeat and Dahlin algorithm:

Manual 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
Velocity PID Cascade
Digital Sampled Data Controller

Objective of this Case Study

The objective of this case study is to explore the design methodology and performance capability of a PI with feed forward controller. An additional objective is to establish some design criteria which must be met if a PI with feed forward control implementation is to provide significant benefit in rejecting unwanted disturbances.

The investigation begins with the Heat Exchanger process, which is studied at two different operating regimes. For both levels of operation, the disturbance rejection capability of a lone PI controller is compared with that of a PI with feed forward controller. An important criterion resulting from this first investigation is that:

1) The success of a feed forward element in rejecting disturbances depends on how well the feed forward dynamic model, which is central to this advanced controller architecture, matches the observed behavior of the process.

This is followed by a second investigation using the Gravity Drained Tanks process. In this investigation, the feed forward dynamic model is shown to very accurately describe the observed behavior of the process but poor disturbance rejection still results. This leads to the second criterion:

2) For a feed forward element to effectively reject disturbances, the dead time of the manipulated input to measured output dynamics must be smaller than the dead time of the disturbance to measured output dynamics.

Feed Forward Control

A feedback controller takes corrective action by adjusting the manipulated input variable, U(t), only when a control error exists (when the measured output variable, Y(t), does not equal the set point, $Y_{SP}(t)$). However, in some processes, a disturbance can occur which does not immediately impact the measured variable. For example, if a disturbance causes a liquid entering a long pipe to unexpectedly increase and the control loop temperature measurement is located at the pipe exit, hot liquid can fill the pipe and build tremendous disruptive momentum before the feedback controller detects the problem and begins corrective action. As this simple example illustrates, feedback controllers simply start too late to be effective in minimizing the impact of some disturbances on the measured variable.

The function of a feed forward element is to begin taking corrective action as soon as a disturbance occurs and *before* it has a chance to impact the measured output variable. As shown in Figure 1, a feed forward element is most often implemented in combination with a feedback controller and consists of two parts:

1) a sensor/transmitter which measures the disturbance variable, and

2) a feed forward model which describes the dynamic interaction among the disturbance, manipulated input and measured output variables.

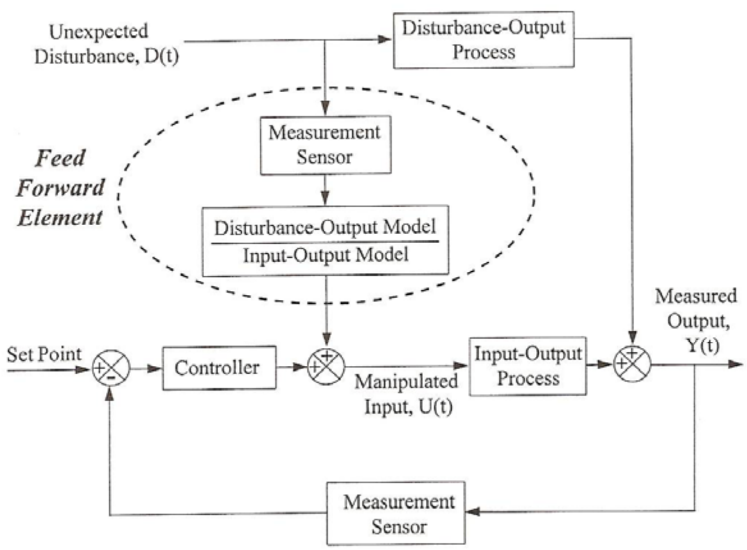

Figure 1. Architecture of a feed forward controller with feedback trim

The feed forward model is fundamental to the architecture of the controller and should reasonably describe the dynamics of the disturbance, D(t), to measured output, Y(t), in ratio to the dynamics of the manipulated input, U(t), to measured output, Y(t). Once online, the sensor measures changes in D(t) and transmits these changes to the feed forward model. The model uses this disturbance signal in computations to determine the corrective U(t) actions which must be taken now to head off the impending disruption of D(t) on Y(t).

In a perfect world, disturbance rejection is complete and Y(t) remains unperturbed. In practice, however, a feed forward controller with feedback trim often mitigates but rarely eliminates the impact of the disturbance on the measured variable. In this case study, some reasons for this imperfect result will be established.

Note that in practice, there are often several disturbance variables which can disrupt production. Since there are costs associated with the implementation of a feed forward element, judgment must be used to select the most profitable applications of this technology.

The Feed Forward Dynamic Model

The following discussion, which presents a logical argument leading to the final form of the feed forward dynamic model, uses Laplace domain variables. Even if the reader is unfamiliar with Laplace transforms, the logic of the discussion can (hopefully) be followed from the presentation.

Let $G_P(s)$ be a mathematical model (transfer function) which describes the dynamics of the manipulated input to measured output variable. Then, when a change in manipulated variable U(s) occurs, its impact on measured variable Y(s) can be computed:

$$Y(s)_{INPUT} = G_P(s)U(s) \tag{1}$$

Similarly, let $G_D(s)$ be a mathematical model which describes the dynamics of the disturbance to measured output variable. That is, when a change in disturbance variable D(s) occurs, its impact on measured variable Y(s) can be computed:

$$Y(s)_{DISTURBANCE} = G_D(s)D(s) \tag{2}$$

Now, suppose a disturbance D(s) occurs which will increase Y(s) by a certain amount. The function of the feed forward model is to compute a change in U(s) which will decrease Y(s) by the same amount, thus canceling the effect of the disturbance on the measured variable. Since the impact of change in the input variable must be opposite to that resulting from the disturbance, then:

$$Y(s)_{INPUT} = -Y(s)_{DISTURBANCE} \tag{3}$$

or using the dynamic models:

$$G_P(s)U(s) = -G_D(s)D(s) \tag{4}$$

which leads to the feed forward dynamic model computation. That is, the change in U(s) which must occur to compensate for changes in D(s) is computed:

$$U(s) = -\frac{G_D(s)}{G_P(s)}D(s) \tag{5}$$

This computation can become rather sophisticated because the gain, time constant and dead time of the input-output model, $G_P(s)$, will most likely be different from that of the disturbance-output model, $G_D(s)$. Thus, a sequence of moves must be computed which counteract the disturbance by appropriate amounts over a period of time.

To compute this sequence in Picles, first order plus dead time (FOPDT) dynamic forms are assigned to the dynamic models:

$$G_P(s) = \frac{K_P e^{-\theta_P s}}{\tau_P s + 1} \quad \text{and} \quad G_D(s) = \frac{K_D e^{-\theta_D s}}{\tau_D s + 1} \tag{6}$$

where K_P and K_D are the steady state gains, τ_P and τ_D are the overall time constants, and θ_P and θ_D are the apparent dead times of the input-output and disturbance-output models respectively. Substituting the model forms of Eq. 6 into the feed forward model of Eq. 5 results in the final form:

$$U(s) = -\frac{K_D}{K_P}\left(\frac{\tau_P s + 1}{\tau_D s + 1}\right)e^{-(\theta_D - \theta_P)}D(s) \tag{7}$$

And thus, when designing a feed forward element in Picles, the user must specify the:

Gain Ratio, K_D/K_P
Process Time Constant, τ_P
Disturbance Time Constant, τ_D
Dead Time Difference, $\theta_D - \theta_P$

Heat Exchanger Investigation #1

The Heat Exchanger process, shown in Figure 2, is a counter-current lube oil cooler. The manipulated variable is the cooling liquid flow rate on the shell side. The measured/controlled variable is lube oil temperature exiting the exchanger on the tube side. This nonlinear process has a negative steady state process gain. That is, as the manipulated cooling flow rate increases, the measured exit temperature decreases.

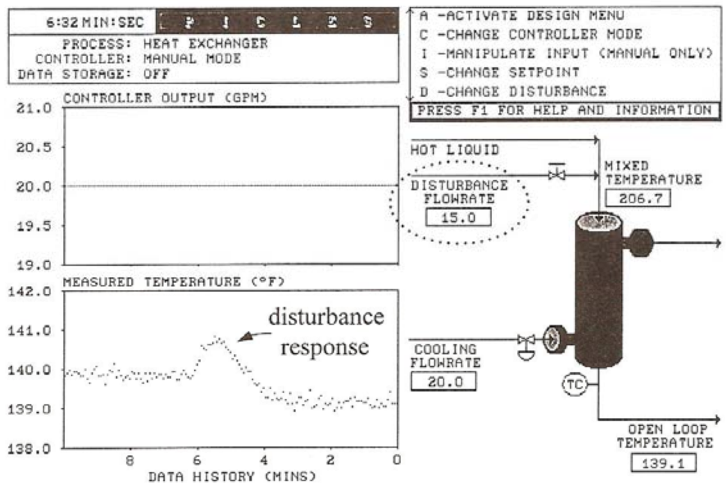

Figure 2. Picles graphic of the Heat Exchanger process shows inverse response to step disturbance

As shown in the measured variable strip chart to the lower left in Figure 2, load disturbances produce an inverse (also called nonminimum phase) open loop response in the measured exit temperature. This is because an increase in the disturbance flow rate both increases the total flow rate of liquid through the exchanger tubes and, since the disturbance stream is cooler than the hot oil liquid stream, also lowers the mixed temperature of the liquid entering the exchanger. Material already in the exchanger when the disturbance first occurs is forced through faster than normal, reducing the time it is exposed to the coolant stream and resulting in a rise in the measured exit temperature. Once the new cooler mixed liquid works its way through the exchanger, however, it steadies out at a cooler exit temperature than prior to the disturbance. Thus, as shown in Figure 2, an increase in the disturbance flow rate causes the measured exit temperature to first rise and then ultimately decrease to a new lower steady state temperature.

Dynamic Modeling and Controller Design Using Digest

The design of the PI controller for all investigations in this case study follows the traditional method of approach as detailed in the popular process control texts:

1) step or pulse the manipulated variable in open loop (manual mode),
2) record the manipulated and measured variable data as the process responds to the step or pulse,
3) fit a low order linear dynamic model to this manipulated to measured variable data,
4) use the linear dynamic model parameters in a correlation to obtain intitial estimates of controller tuning parameters,
5) implement this controller (close the loop) and evaluate its performance, and
6) perform a final tuning by trial and error until desired controller performance is obtained.

Digest is a user friendly tool for quickly and easily performing steps 3 and 4 above. Digest can import files containing dynamic data from Picles, from 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 input variable data, the measured output 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 sampling rate is constant.

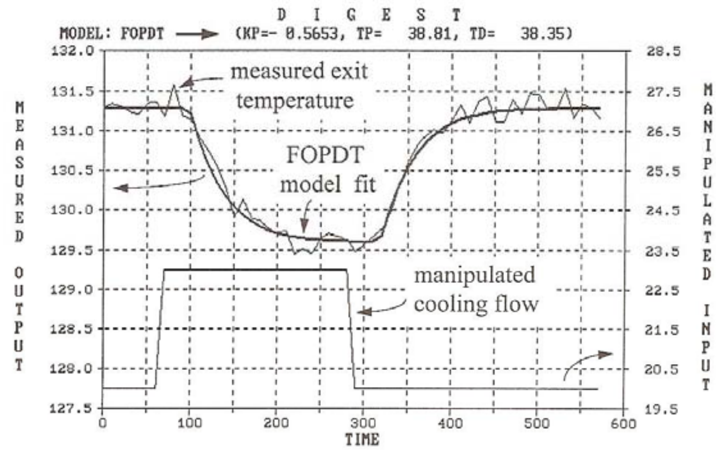

Figure 3. Digest fit of a FOPDT dynamic model to input-output pulse test data

This first investigation occurs at an operating regime where the manipulated cooling flow rate is steady at 20 gpm (gallons per minute) and the disturbance flow rate is steady at 45 gpm. These conditions are chosen because the inverse portion of the disturbance response is very small at this operating level and as a result, a FOPDT dynamic model will accurately represent the data.

Following the controller design procedure, the manipulated cooling flow rate is pulsed from the initial steady value of 20 gpm up to 23 gpm, and about 210 seconds later, back down to 20 gpm. Picles' file storage utility is used to save the data to disk. Figure 3 shows that the FOPDT model fit by Digest accurately describes the pulse test data. As indicated at the top of the figure, the parameters computed by Digest for this manipulated input to measured output model are:

Process Gain, $K_P = -0.565\ ^{O}F/gpm$
Overall Time Constant, $\tau_P = 38.8$ seconds
Apparent Dead Time, $\theta_P = 38.4$ seconds

These dynamic model parameters are now used in one of several 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. Figure 4 shows such a computation for the above FOPDT model parameters for a PI controller.

In this case study, ITAE for Disturbance Changes tuning is used. Note that equally logical choices are the IAE for Disturbance Changes tuning or the IMC tuning. Circled in Figure 4 are the ITAE tuning parameters computed by Digest:

Controller Gain, $K_C = -1.54\ gpm/^{O}F$
Reset Time, $\tau_I = 57.1$ seconds

```
Controller Mode: PI

        Internal Model Control (IMC)
TC (Closed Loop Time Constant) =    30.68
Controller Gain = -  0.995
Reset Time      =    38.81
             Cohen-Coon
Controller Gain = -  1.759
Reset Time      =    43.95
        ITAE (for Set Point Changes)
Controller Gain = -  1.048
Reset Time      =    44.76
       ITAE (for Disturbance Changes)
Controller Gain = -  1.537
Reset Time      =    57.11
       IAE (for Set Point Changes)
Controller Gain = -  1.355
Reset Time      =    55.37
       IAE (for Disturbance Changes)
Controller Gain = -  1.761
Reset Time      =    63.29
```

Figure 4. ITAE for Disturbance Changes PI tuning parameters computed by Digest for the FOPDT parameters of Figure 3

The Feed Forward Element

Before testing the PI controller on the process, which is the next step in the design procedure listed earlier, the design of the feed forward element is completed. This is accomplished by pulsing the disturbance flow rate from its initial steady value of 45 gpm up to 50 gpm, and about 210 seconds later, back down to 45 gpm.

Note that when modeling this data in Digest, the disturbance flow rate data must be labeled as the manipulated input variable and the exit temperature as the measured output variable. As shown in Figure 5, the inverse response behavior discussed earlier and shown in Figure 2 is minimal at this operating regime, so a FOPDT model quite reasonably describes the data. Indicated at the top of Figure 5 and listed below are the model parameters for this disturbance to measured output model:

Disturbance Gain, $K_D = -0.253\ ^{o}F/gpm$
Disturbance Time Constant, $\tau_D = 30.6$ seconds
Disturbance Dead Time, $\theta_D = 52.0$ seconds

Using this manipulated input to measured output model and disturbance to measured output model, the feed forward model parameters to be entered into Picles are computed:

Gain Ratio, $K_D/K_P = 0.45$
Process Time Constant, $\tau_P = 38.8$ seconds
Disturbance Time Constant, $\tau_D = 30.6$ seconds
Dead Time Difference, $\theta_D - \theta_P = 13.6$ seconds

Comparing the Controllers

Returning to Picles, the disturbance rejection capability of the PI controller is compared with that of the PI with feed forward controller. This comparison is shown in the strip chart of Figure 6. In Picles and in most commercial systems, a PI controller is implemented by selecting a PID form and then setting the derivative time tuning parameter to zero.

The disturbance is traced in Figure 6 across the lower portion of the strip chart and is shown to step in two square wave pulses between 45 and 50 gpm. The set point and measured exit temperature traces are displayed across the upper portion of the chart. As shown, the set point remains constant throughout the test as the focus of this controller design is on disturbance rejection.

The left portion of the strip chart shows the disturbance rejection capability of the PI controller when tuned using the ITAE settings from Figure 4. As can be seen in Figure 6, the PI controller alone is not capable of rejecting the disturbance as both the disturbance step up and the step back down on the left side of the chart have a large impact on the measured exit temperature.

The right portion of Figure 6 shows the disturbance rejection capability of the PI with feed forward controller. When the disturbance flow is pulsed in the same manner as before, the feed forward element quite successfully minimizes the impact of the disturbance on the measured exit temperature.

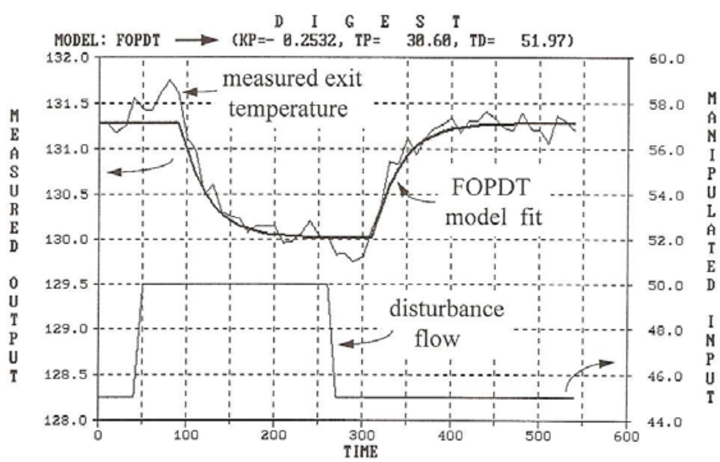

Figure 5. Digest fit of a FOPDT dynamic model to disturbance pulse test data

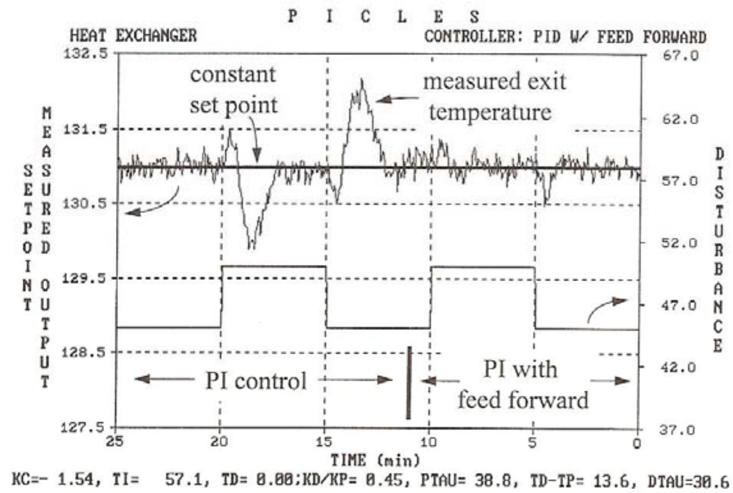

Figure 6. Disturbance rejection capability of a PI controller (left) and a PI with feed forward controller (right)

Heat Exchanger Investigation #2

In investigation #1, both the input-output and the disturbance-output FOPDT models reasonably described the pulse test data. The feed forward element which was designed using parameters from these models was shown to substantially reject disturbance pulses before they could impact the measured exit temperature.

This second investigation explores the benefits of the feed forward element when the dynamic model does not reasonably describe the observed behavior of the disturbance response. The operating regime for this second investigation begins with the manipulated cooling flow rate again being steady at 20 gpm. The difference here is that the disturbance flow rate is steady at the much lower value of 12 gpm. At these conditions, changes in the disturbance flow rate produce a significant inverse response in the measured exit temperature.

Dynamic Testing

Rather than pulse testing to generate dynamic data for modeling, this second investigation employs step testing. Both pulse and step tests are acceptable methods for generating dynamic data and each is used in this case study to illustrate the point.

Similar to the procedure used in the first investigation, the manipulated cooling flow rate is stepped from the initial steady value of 20 gpm up to 21 gpm. Picles' file storage utility is used to save the data to disk. As shown in Figure 7, the FOPDT model fit by Digest accurately describes the test data and as indicated at the top of the figure, the parameters for this manipulated input to measured output model are:

Process Gain, K_P = - 1.07°F/gpm
Overall Time Constant τ_p = 61.0 seconds
Apparent Dead Time, θ_p = 46.8 seconds

Using these dynamic model parameters and again choosing the ITAE for Disturbance Changes tuning correlation, the PI tuning parameters computed by Digest are:

Controller Gain, K_C = - 0.23 gpm
Reset Time, τ_I = 50.0 seconds

The Feed Forward Element

To generate dynamic data for the design of the feed forward element, the disturbance flow rate is stepped from its initial steady value of 12 gpm up to 15 gpm. The dynamic response is shown both in the strip chart to the lower left in Figure 2 and also in Figure 8. The large inverse response is apparent in both figures and the FOPDT fit from Digest shown in Figure 8 does not completely describe the observed dynamic behavior.

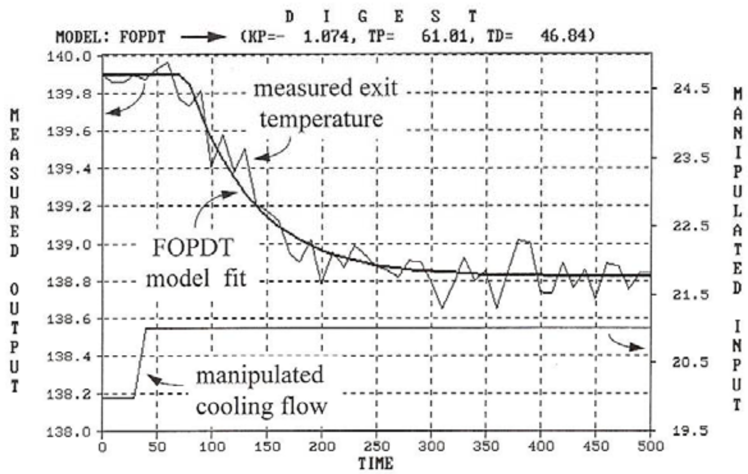

Figure 7. Digest fit of a FOPDT dynamic model to input-output step test data

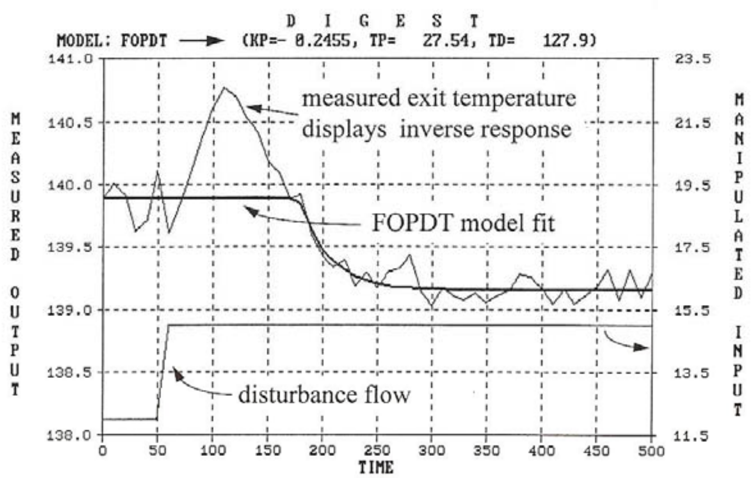

Figure 8. Digest fit of a FOPDT dynamic model to disturbance step test dat exhibiting a large inverse response

The lowest order model which can reasonably describe the data in Figure 8 is probably a second order plus dead time with lead element dynamic form. Unfortunately, Picles only permits entry of FOPDT model parameters in the feed forward controller tuning page. This limitation, due to the options in Picles and rather than a limitation of the theory, provides a good opportunity to explore the importance of model accuracy as it affects feed forward controller performance.

Before continuing, a comment in defense of the FOPDT model form: in most cases, the FOPDT model accurately describes the change in steady state (the gain) and the speed of response in the data (the overall time constant), although in this case the tracking starts after the inverse portion of trajectory. Also, a FOPDT model usually provides a good approximation of dead time, and even though the entire inversion portion of the response is approximated here as one large dead time, this approximation is entirely appropriate when modeling inverse response input-output data to design a traditional PID feedback controller.

In any event, as indicated at the top of Figure 8 and listed below are the model parameters for this disturbance to measured output FOPDT model:

Disturbance Gain, $K_D = -0.246$°F/gpm
Disturbance Time Constant, $\tau_D = 27.5$ seconds
Disturbance Dead Time, $\theta_D = 128$ seconds

Using the manipulated input to measured output model and disturbance to measured output model, the feed forward model parameters to be entered into Picles are computed:

Gain Ratio, $K_D/K_p = 0.23$
Process Time Constant, $\tau_p = 61.0$ seconds
Disturbance Time Constant, $\tau_D = 27.5$ seconds
Dead Time Difference, $\theta_D - \theta_p = 81.1$ seconds

Comparing the Controllers

Returning to Picles, the disturbance rejection capability of the PI controller is compared with that of the PI with feed forward controller. This comparison is shown in the strip chart of Figure 9. As before, the disturbance is traced across the lower portion of the strip chart, and in this investigation, the disturbance is stepped in two square wave pulses between 11 and 15 gpm. The set point and measured exit temperature traces are displayed across the upper portion of the chart. The set point remains constant throughout the test.

The left portion of the strip chart shows the disturbance rejection capability of the PI controller when tuned using the ITAE settings listed above. As before, the PI controller alone is not capable of rejecting the disturbance as both the disturbance step up and the step back down on the left side of the chart have a large impact on the measured exit temperature. It is interesting to further observe how the character of the disturbance rejection is so much different in Figure 9 for the one PI controller than was observed in Figure 6, especially when considering that both investigations are for the same heat exchanger process.

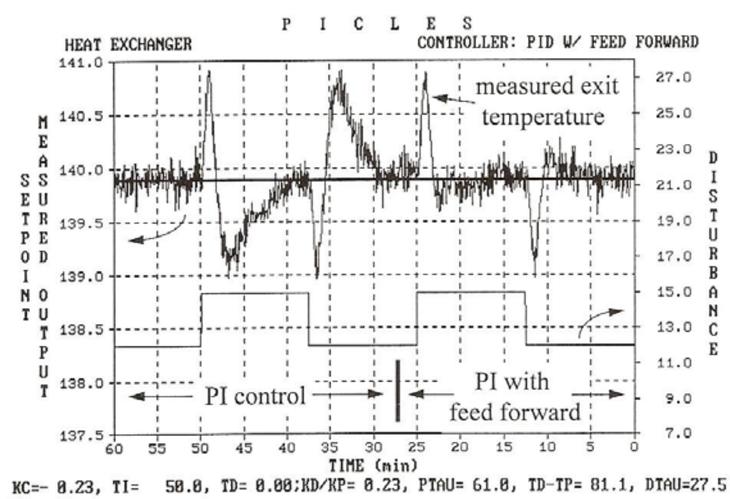

Figure 9. Disturbance rejection capability of a PI controller (left) and a PI with feed forward controller (right)

The right portion of Figure 9 shows the disturbance rejection capability of the PI with feed forward controller. When the disturbance flow is pulsed in the same manner as before, the impact of the poor match between the FOPDT model and the disturbance response data shown in Figure 8 is apparent. The feed forward element is successful in dampening the transient caused by the disturbance faster than the lone PI controller. However, it is not able to completely reject the disturbance, as spikes in the measured exit temperature in response to each disturbance step are clearly evident.

Design Criteria #1

A comparison of Figure 6 and Figure 9 highlights the importance of the first design criteria for successful implementation of a feed forward controller with feed back trim:

1) The success of a feed forward element in rejecting disturbances depends on how well the feed forward dynamic model, which is central to this advanced controller architecture, matches the observed behavior of the process.

Gravity Drained Tanks Investigation

The Gravity Drained Tanks process, shown in Figure 10, consists of two non-interacting gravity drained tanks in series. The manipulated input variable for this process is the flow rate of liquid entering the top tank. The measured/controlled output variable is liquid level in the lower tank. The disturbance variable is a secondary flow out of the lower tank due to a positive displacement pump. Thus, the disturbance flow is independent of liquid level except when the tank is empty. This process is modestly nonlinear because the drain rate from each tank is proportional to the square root of the hydrostatic head (liquid level in the tank).

Dynamic Testing

This third investigation occurs at an operating regime where the manipulated inlet flow rate is steady at 20 cm^3/sec and the disturbance flow rate is steady at 5 cm^3/sec. Following the established procedure, the manipulated inlet flow rate is briefly pulsed down to 18 cm^3/sec. As shown in Figure 11, the FOPDT model fit by Digest very accurately describes the test data and as indicated at the top of the figure, the parameters for this manipulated input to measured output model are:

Process Gain K_p = 4.58 cm/(cm^3/sec)
Overall Time Constant, τ_p = 88.1 seconds
Apparent Dead Time θ_p = 33.0 seconds

Using these dynamic model parameters in the ITAE for Disturbance Changes tuning correlation, the PI tuning parameters computed by Digest are:

Controller Gain, K_c = 0.33 (cm^3/sec)/cm
Reset Time τ_I = 88.1 seconds

The Feed Forward Element

To generate dynamic data for the design of the feed forward element, the disturbance flow rate is briefly pulsed from its initial steady value of 5 cm^3/sec up to 7 cm^3/sec. As shown in Figure 12, the FOPDT model fit by Digest also very accurately describes the test data and as indicated at the top of the figure, the parameters for this disturbance to measured output model are:

Disturbance Gain, K_D = -4.63 cm/(cm^3/sec)
Disturbance Time Constant, τ_D = 48.6 seconds
Disturbance Dead Time, θ_D = 2.3 seconds

Using the manipulated input to measured output model and disturbance to measured output model, the feed forward model parameters to be entered into Picles are computed:

Gain Ratio, K_D/K_p = -1.01
Process Time Constant, τ_p = 88.1 seconds
Disturbance Time Constant, τ_D = 48.6 seconds
Dead Time Difference, $\theta_D - \theta_p$ = 0.0 seconds

Based on the FOPDT model parameters, the dead time difference is negative (-30.7 seconds). However, it is entered into Picles as zero. *This is not a limitation of Picles, but rather, is consistent with the underlying theory.* If negative dead time differences were permitted, this would require that the feed forward model use future values of the disturbance variable in its calculations, which for practical implementations, are impossible to know. The minimum dead time difference permitted by the theory is zero, requiring that the feed forward model use the most recent disturbance measurement in its calculation.

The strip charts shown in Figure 10, which show the Gravity Drained Tanks under PI with feed forward control, permit a visual appreciation of this idea. The bottom strip chart shows the measured level in the lower tank. The top strip chart shows the output of a PI with feed forward controller. As these charts reveal, the instant that the disturbance flow rate increases, the measured level begins to fall. The feed forward element takes immediate action (a zero delay in decision making) and jumps the inlet flow rate to mitigate the impact of the disturbance.

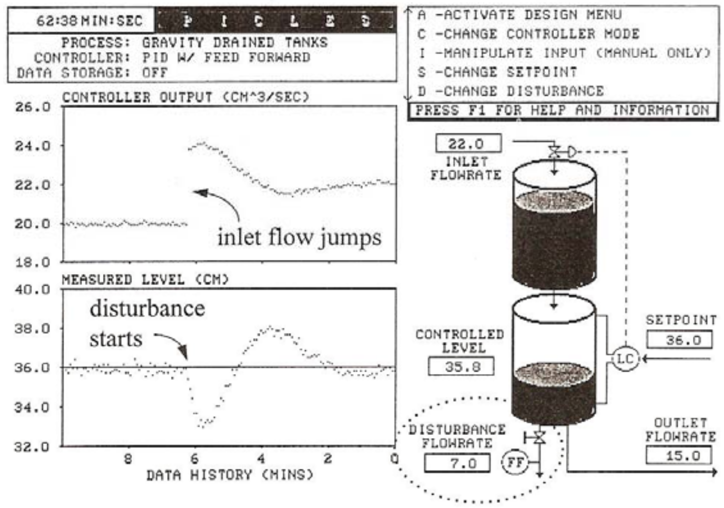

Figure 10. Picles graphic of the Gravity Drained Tanks process shows impact of feed forward element on controller output

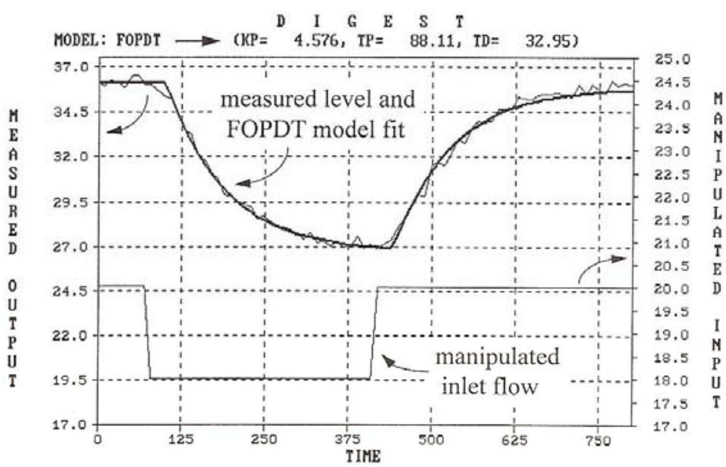

Figure 11. Digest fit of a FOPDT dynamic model to input-output pulse test data

A Feed Forward Failure?

Returning to Picles, the disturbance rejection capability of the PI controller is compared with that of the PI with feed forward controller. This comparison is shown in the strip chart of Figure 13. Again, the disturbance is traced across the lower portion of the strip chart and is stepped in two square wave pulses between 5 and 7 cm^3/sec. The set point and measured exit temperature traces are displayed across the upper portion of the chart with the set point remaining constant throughout the test.

As is evident in Figure 13, the feed forward controller changes the shape of the closed loop response but is unable to reduce the overall impact of the disturbance on the measured level. This is in spite of the fact that both FOPDT models very accurately describe the dynamic data and that the feed forward controller takes a large and immediate action to mitigate the disturbance as shown in Figure 10.

An intuitive appreciation for this feed forward "failure" can be obtained from the process graphic shown in Figure 10. The disturbance is a flow out of the bottom of the lower tank. When this disturbance flow rate increases, the measured level in the lower tank immediately begins to fall. In response, the feed forward controller immediately increases the manipulated flow rate into the top tank.

For this inlet flow rate increase to impact the level in the lower tank, however, it must persist long enough such that the level in the top tank begins to rise. This in turn causes the drain rate out of the top tank and into the lower tank to rise, which then finally begins to raise the measured level in the lower tank. In short, the disturbance rejection failure occurs because the dead time of the manipulated input to measured output dynamics is significantly longer than the dead time of the disturbance to measured output dynamics.

Design Criteria #2

This last investigation, where the feed forward dynamic model is shown to closely match the observed behavior of the process yet poor disturbance rejection is observed, leads to the second important feed forward element design criterion:

2) For a feed forward element to effectively reject disturbances, the dead time of the manipulated input to measured output dynamics must be smaller than the dead time of the disturbance to measured output dynamics.

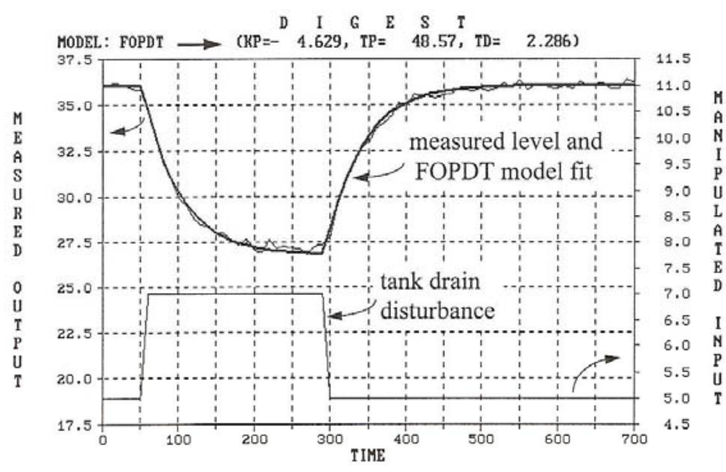

Figure 12. Digest fit of a FOPDT dynamic model to disturbance pulse test data

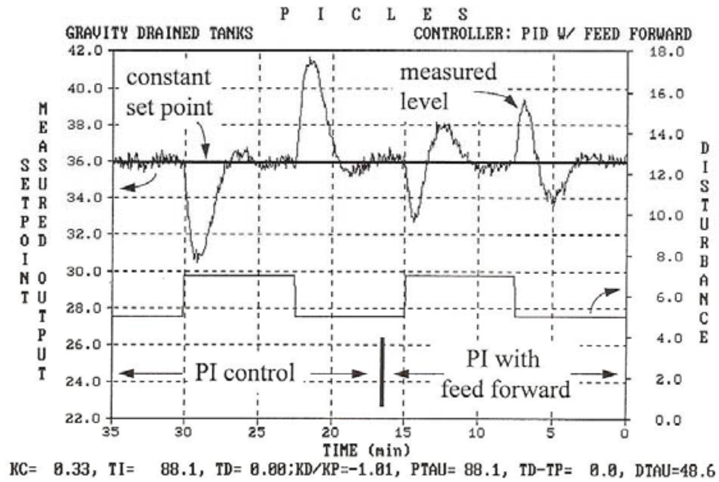

Figure 13. Disturbance rejection capability of a PI controller (left) and a PI with feed forward controller (right)

Homework

The feed forward controller is fickle indeed, but this case study has only explored a few of the issues. Presented was a stark example of the importance of relative dead times on the capability of a PI with feed forward controller. A related issue to explore is the benefit of feed forward control when the overall time constant of the manipulated input to measured output dynamics is much larger than the overall time constant of the disturbance measured dynamics. This concept can be studied in Picles using the Design a Process facility.

Another issue to study using Picles is the relative capability of a static feed forward element, which employs only the gain ratio, as compared to the dynamic feed forward element explored here. A parameter sensitivity case study might explore how controller performance is impacted by errors in the feed forward model gains, time constants or dead times.

For More information

Picles and Digest offer tremendous opportunities for "virtual world" learning. For more information about Picles, Digest and available teaching materials, contact:

Doug Cooper
Chemical Engineering Department
University of Connecticut, U-222
Storrs, CT 06269-3222

Phone: (860) 486-4092
E-mail: cooper@eng2.uconn.edu
http://www.eng2.uconn.edu/cheg/picles.html

Acknowledgments

I would like to acknowledge the student program architects who have helped make Picles possible. These include Jerry Bieszczad, Allen Houtz, Robert Schlegel and Adam Lalonde.

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FOUNDATIONS OF COMPUTER-AIDED PROCESS DESIGN

The most recent conference on the Foundations of Computer Aided Process Design (FOCAPD '94) was held in July 1994 at Snowmass, Colorado, under the sponsorship of the CACHE Corporation and the CAST Division of AIChE. The conference brought together 144 engineers and scientists from universities, industry, and government laboratories from 17 countries in order to assess and critique the current status and future directions of computer-aided process and product engineering.

All of the 20 plenary papers (as detailed below) and the 31 contributed papers have been collected together in one volume that is now available from the AIChE Customer Service Department, 345 East 47th Street, New York, NY 10017 (1-800-242-4363). Ask for ISBN 0-8169-0666-1. The price is $75.00 and $60.00 for members.

Contents

Development of an Undergraduate Course Web Site

By Scott Fogler and James C. Piana
The University of Michigan

Introduction

The World Wide Web (WWW) is becoming increasingly recognized by the academic community as a tool for the dissemination of educational materials, over both long and short distances. The hypertextual and graphical capabilities of web browsers such as Netscape coupled with the ready availability of such programs to university students make the WWW an ideal way to present a broad range of materials to students outside of the traditional classroom context.

Near the end of 1995, we began the development of an educational WWW site for the undergraduate chemical reaction engineering course at the University of Michigan. The task facing us was to provide students with a convenient and simple way to access important information, announcements, and other materials for the reaction engineering class. Now, midway through the term, we wish to share a brief overview of our WWW development experiences so far.

WWW Site Content Overview

Since January, 1996, reaction engineering students at the University of Michigan have been using the WWW extensively as a learning tool and information resource. All course materials that have traditionally been handed out to students or placed on reserve in the engineering library are now posted on the Internet. The materials available to students include the following:

- Course Syllabus
- Homework Solutions
- Lecture Reviews
- Student Grades
- Review Material
- Photos of Industrial Chemical Reactors

Also included is a substantial amount of new material from the forthcoming third edition of Fogler's "Elements of Chemical Reaction Engineering." Much of the new third edition material is required reading for the students in the reaction engineering class, and some not-yet-published end of chapter problems have been posted on the Internet and given as homework assignments. Students have access to the Web pages from any computer lab on campus or from their own personal computers at home, and can obtain a printout of any of the material using the print command of their web browser.

Development of the WWW Site

In the first few weeks of the term, the web site quickly grew from a small number of pages organized from a single main menu to a large collection of sections, comprised of over 1,000 files totaling more than 20MB. The development of an easy-to-use and aesthetically pleasing interface for the student became a high priority. The current version of the user interface brings the student first to a main menu that lists all the sections of available information. The use of a clickable map, shown in Figure 1, provides a good overview of the content of the site, and makes it very easy for the student to jump to a specific section.

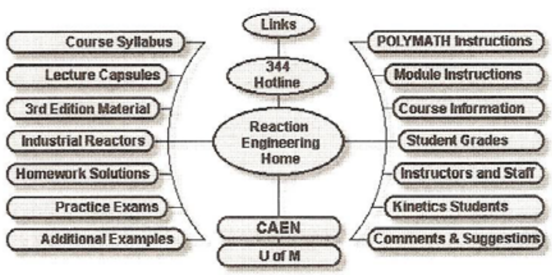

Figure 1. The Reaction Engineering Web Site Main Menu

As for navigation from section to section, we followed the general rule of Web site design that nothing should be more than two or three links (mouse clicks) away from anything else. This ease of navigation is accomplished in a few different ways. First, at the bottom of each Web page, there is a clickable button bar that links the student to each of the main sections of the site (see Figure 2).

Figure 2. Button Bar

A site index provides a comprehensive list of topics from which the student may select a topic and jump directly to the relevant information or menu. Many pages also contain direct links to other section of the Web site, encouraging student exploration of each individual section. Finally, a standard page format is used for the majority of the Web pages to lend a sense of continuity as a student navigates through the site.

Creating and editing the content of the site has been the most time-consuming aspect of our development activities. There are many different methods of converting documents to WWW format, and the selection of the conversion method depends primarily on the content of the document as well as the format in which the document is available. For documents with only hard copy available, conversion generally involves the use of an optical scanner. If the document is text-only (text-only is taken here to mean that the document contains no graphics or equations), it can be scanned as text (using optical character recognition software) and saved as a text file. This text file must then be edited with Hypertext Markup Language (HTML) formatting tags to convert the document into a browser-readable page. If the document contains pictures and/or equations (such as a textbook page or a homework solution) the images must be scanned separately, edited, and saved as an image file that is then included in the Web page. For documents that are available as a word processor file, graphical elements are easily removed from the word processor document and converted to a Web compatible image file. This saves a great deal of time over scanning the images, as the scanning and image editing steps are eliminated. There are also many different shareware programs that can convert files from popular commercial word processors directly to HTML files, but we have had very little luck using these programs due to the complexity of the source word processor files.

Student Reaction

As with any new addition to a course, student reaction to the Reaction Engineering web pages has been mixed. Students like the availability of the material on the Web, have reported no difficulties in accessing the site, and have commented that the Web material reinforces and enhances the lectures and assigned readings. Early on, students complained that many of the equations, especially those with very small subscripts and italic type, were difficult to read on printed copies of the Web material. We easily remedied this situation by increasing the font size and removing any italics from the equations. The only significant student complaint we have yet to address is the length of time it takes to print the Web pages on the networked campus computers. Pages that contain more than one or two graphical element (equations, figures, and scanned images) take several minutes to print, leading to long print queues and short tempers in the student labs. As a temporary fix, we have placed clean copies of all the material on reserve in the library. We are now working to find a simple way to decrease the printing time so we can do away with the reliance on the reserve desk altogether.

Conclusions (Thus Far)

At this point in the term, we have found that the use of the Web site in the undergraduate reaction engineering class has not only been an effective method of providing students with easy access to the course materials, but it has also been an easy way to communicate with the students outside of the classroom. Since changes in assignments and other announcements can be made at any time on the Web pages, we do not have to wait for the next scheduled lecture to pass information along to the students. While this of course depends on student use of the Web, this is an added benefit of the use of the Web as an instructive tool.

Future directions for the Web site will be guided both by student comments and suggestions, and by the expanding capabilities of web browser software. As the interactive capabilities of Internet software grow, we expect to find new and useful applications of the WWW both in the classroom and beyond.

Where to Find the Site

If you would like to pay a visit to the Reaction Engineering home page, the URL is http://www.engin.umich.edu/labs/mel/class/kinetics.html. Please do not hesitate to send any comments or suggestions to:

Scott Fogler
Department of Chemical Engineering
The University of Michigan
3168 H.H. Dow Building
Ann Arbor, MI 48109-2136
Phone: (313) 763-1361
sfogler@engin.umich.edu

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 delayed version of POLYMATH 4.0 should be available by June 1st. All site-license users will automatically get this updated version as soon as it is released, and **no special request is necessary.** Users who need a beta version of Polymath 4.0 should contact Michael Cutlip at MCUTLIP@Uconnvm.Uconn.Edu. 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:

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

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New CACHE Trustee

Ross Taylor

Ross is a Professor of Chemical Engineering at Clarkson University in Potsdam, New York where he has been since 1980. He received his B.Sc, M.Sc and Ph.D degrees from the University of Manchester, Institute of Science and Technology in England. He is a coauthor (with Professor R. Krishna of the University of Amsterdam) of Multicomponent Mass Transfer (Wiley, 1993) and with Harry Kooijman of ChemSep, a software package for simulating multicomponent separation processes which features a mass transfer rate based column simulation model. (ChemSep has been a CACHE product since 1993) He holds an appointment as a visiting professor from the OSPT (an organization of Chemical Engineering Departments in The Netherlands) for whom he regularly teaches short courses.

Ross and his wife Elizabeth have four children: Julie, Jeremy, Andrew and Claudia. During the all too brief North Country summers he can often be found coaching youth soccer teams involving one or another of his children.

1998 Conference Announcement

FOUNDATIONS OF COMPUTER AIDED PROCESS OPERATIONS (FOCAPO III)

Area 10C of the AIChE Programming Committee has approved the co-sponsorship with CACHE of FOCAPO III to be held in the summer of 1998. The first conference was held in Park City, Utah in 1987 and the second conference took place in Crested Butte, Colorado in July, 1993.

Since that time the interest in process operations has, if anything, further increased. Few new large chemical plants are being designed and built, at least in Europe and North America. For existing plants, flexibility and responsiveness in operation are the order of the day. Continually developing computing capabilities allow ever more demanding targets for flexibility and responsiveness to set the competitive agenda both nationally and internationally within the process industries and between these and other industries.

The objectives of FOCAPO III will review progress since the last conference both in academic work to develop tools for this field and in the state of industrial applications. Important issues to be examined include how to implement more effective interaction between industry and universities on operational problems and how to identify significant new problem areas. These concepts will set the agenda for integrating the various techniques and sub-themes of operations into a common framework defining a new discipline of process operations.

Contact the co-chairs if you have some suggestions for the program:

Gary D. Cera
Mobil Oil Corp.
Paulsboro Refinery
800 Billingsport Road
Paulsboro, NJ 08066
(609) 224-2336

Joseph F. Peckney
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907-1283
(317) 494-7901
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