CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

No. 43 FALL 1996

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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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CACHE NEWS

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66-444
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CACHE NEWS

No. 43 Fall 1996

Nonideal Reactor Design Using POLYMATH 4.0

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

One of the convenient new features in POLYMATH provides for the use of logical variables during the solution of algebraic and differential equations. This is discussed in this article in the context of Chemical Reaction Engineering where the design of nonideal reactors is being considered. This article also suggests interesting techniques for comparison of graphical results when various cases involving ordinary differential equations are considered.

Simulation of Nonideal Reactors with Segregated Flow

Nonideal reactor design for segregated flow involves the solution of

$$\bar{C}_A = \int_0^\infty E(t) C_A(t)\, dt \qquad (1)$$

where E(t) is the residence time distribution function (RTD) and $C_A(t)$ is the concentration from a batch reactor at time t.

$\bar{C}_A$ is the calculated outlet concentration.

The above integral equation can be written in differential equation form as

$$\frac{d\bar{C}_A}{dt} = E(t) C_A(t) \qquad \text{I. C. } = 0 \text{ at } t = 0 \qquad (2)$$

for evaluation by POLYMATH when the E(t) function is known. Integration is carried out to large values of t where the resulting outlet concentration $\bar{C}_A$ no longer changes with time.

For a laminar flow reactor the RTD is given by $E(t) = \frac{\tau}{2t^3}$ when $t \geq \frac{\tau}{2}$ else it is zero. Here τ (tau) is the mean residence time of the reactor given by V/v_0. The RTD function for laminar flow can be entered using the POLYMATH if, then, else logical variable statement.

EoftLAMINAR=if(t>=tau/2.)then(tau^2/(2.*t^3))else(0.0)

Let us consider a second order, irreversible, liquid phase reaction occurring within the laminar flow reactor using the RTD function. This can easily be handled in POLYMATH by numerically solving the differential equation for the batch reactor given by

$$\frac{dC_A}{dt} = -kC_A^2 \qquad \text{I. C. } C_A = 1.0 \text{ at } t = 0 \qquad (3)$$

during the simultaneous integration of the RTD differential equation (2) for $\bar{C}_A$. This example is for the initial concentration of C_A to be 1.0.

The POLYMATH equations for the case where k=0.2 and tau = 5.0 are shown below in Figure 1 as they appear on the screen prior to solution.

```
        RTD Treatment for a 2nd Order Reaction in a Laminar Flow Reactor
Equations                                                    Initial values
  d(CABATCH)/d(t)=-k*CABATCH^2                               1
  d(CALAMINAR)/d(t)=EoftLAMINAR*CABATCH                      0
  k=.2
  tau=5.
  EoftLAMINAR=if(t>=tau/2.)then(tau^2/(2.*t^3))else(0.0)
→ t0 = 0,    tf = 30
```

Figure 1 - Polymath Code for Laminar Flow Reactor

The scaled and titled POLYMATH plot for the laminar flow reactor is shown in Figure 2. Note that the calculated concentration is approaching a constant value at t = 30.

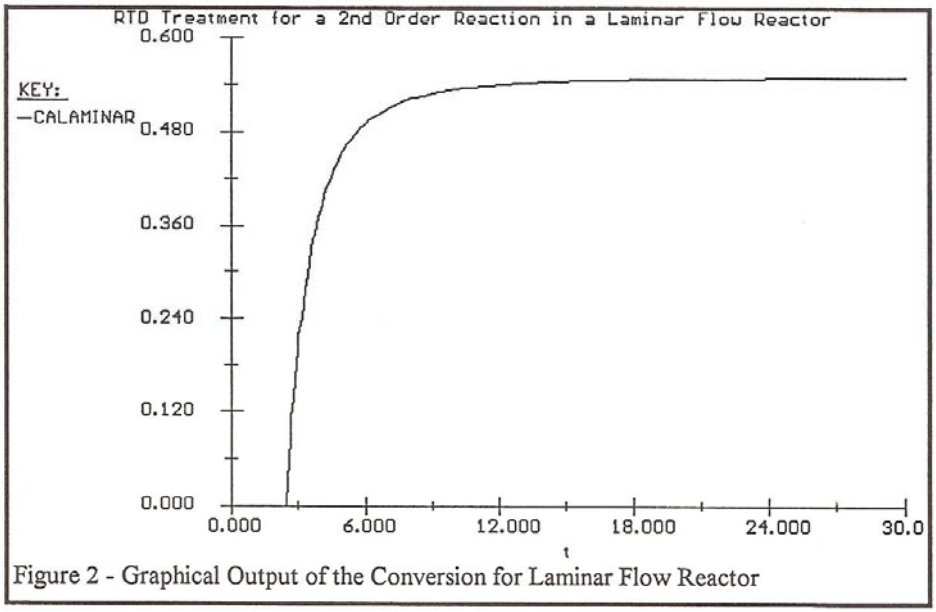

Figure 2 - Graphical Output of the Conversion for Laminar Flow Reactor

The RTD curve for the laminar flow reactor can also be plotted after the numerical solution has been obtained. This is shown in Figure 3 which nicely indicates the breakthrough of the RTD curve at one half of the mean residence time where t = 2.5.

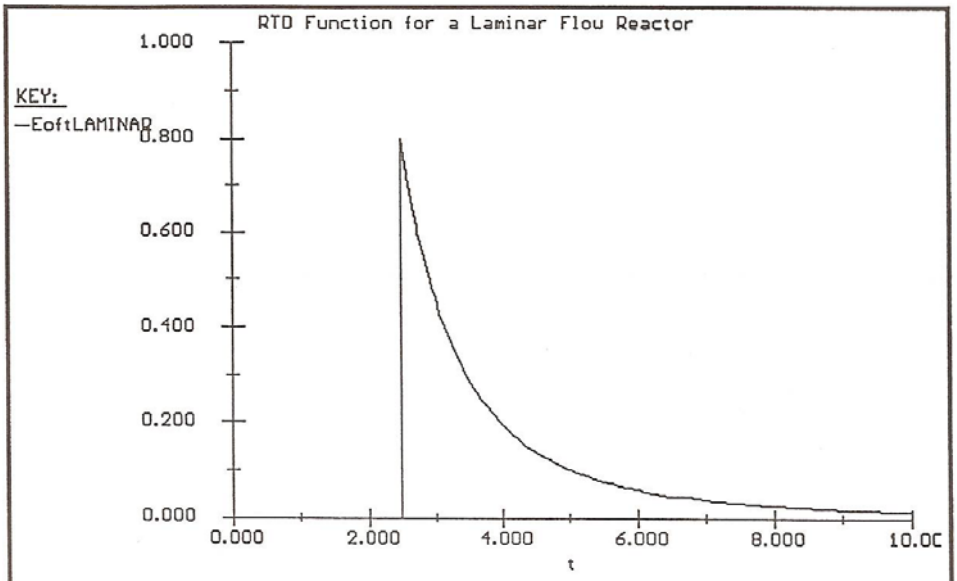

Figure 3 - RTD for Laminar Flow Reactor

This simple example illustrates the usefulness of the logical variable capability with POLYMATH. This problem involving segregated flow modeling can easily be expanded to include the RTD functions for various ideal reactors and experimental RTD's for real reactors as polynomial expressions.

How to Compare Simulations Easily within POLYMATH

The previous example can be extended to other reactors when the RTD functions are known or can be measured. Some of the commonly used ideal reactor RTD's for the plug flow, CSTR and series of N CSTR's can be expressed as:

EoftPLUG=if(t=.99*tau)&(t<1.01*tau))then(1./(tau*2.*(1-.99)))else(0.0)
where this function approaches a dirac delta function at tau = 1.

EoftCSTR=exp(-t/tau)/tau

EoftNCSTR=(t^(N-1)/tau^N/(N-1)!*exp(-t*N/tau)
where N is number of CSTR's in series

The POLYMATH entry for all of the discussed RTD functions is shown in Figure 4 for the case where k = 0.2, tau = 5.0 and N = 10 to a time of t = 30.0.

```
RTD 2nd Order Reaction for Plug Flow, CSTR, N-CSTR, Laminar Flow
Equations                                                    Initial values
  d(CAPLUG)/d(t)=EoftPLUG*CABATCH                            0
  d(CABATCH)/d(t)=-k*CABATCH^2                               1
  d(CALAMINAR)/d(t)=EoftLAMINAR*CABATCH                      0
  d(CACSTR)/d(t)=EoftCSTR*CABATCH                            0
  d(CANCSTR)/d(t)=EoftNCSTR*CABATCH                          0
  k=.2
  tau=5.
  N=10
  EoftPLUG=if((t)=.99*tau)&(t<1.01*tau))then(1./(tau*2.*(1.-.99)))else
     (0.0)
  EoftLAMINAR=if(t)=tau/2.)then(tau^2/(2.*t^3))else(0.0)
  EoftCSTR=exp(-t/tau)/tau
  EoftNCSTR=(t^(N-1)/tau^N)*N^N/(N-1)!*exp(-t*N/tau)
→ t0 = 0,    tf = 30
```

Figure 4 - RTD Treatment for Various Ideal Reactors with Second Order Reaction

The Partial Results Table from the POLYMATH solution shown in Figure 5 which gives general information on various problem variables before the user is prompted for various plots or tabular output.

RTD 2nd Order Reaction for Plug Flow, CSTR, N-CSTR, Laminar Flow

Variable	Initial value	Maximum value	Minimum value	Final value
t	0	30	0	30
CAPLUG	0	0.500004	0	0.500004
CABATCH	1	1	0.142857	0.142857
CALAMINAR	0	0.54862	0	0.54862
CACSTR	0	0.596033	0	0.596033
CANCSTR	0	0.512182	0	0.512182
k	0.2	0.2	0.2	0.2
tau	5	5	5	5
N	10	10	10	10
EoftPLUG	0	10	0	0
EoftLAMINAR	0	0.8	0	0.000462963
EoftCSTR	0.2	0.2	0.00049575	0.00049575
EoftNCSTR	0	0.263511	0	4.86362e-16

Figure 5 - Partial Results Table Generated by POLYMATH

The graphical results of all four reactors are presented in Figure 6 as generated directly by POLYMATH. Note that the solution does not change for times greater than 30 where the solution for each of the various reactors is asymptotically approached. Thus summarized values of the predicted outlet concentrations given in Figure 5 are reasonable. Of course, the integration could be continued to larger time to confirm this. As expected, the calculated concentrations decrease according to the reactor types - CSTR, Laminar Flow, N-CSTR, and Plug Flow. The conversion increase according to the same order. Note that the N-CSTR with N = 10 approaches that of the Plug Flow reactor. This could also be calculated with larger values of N by rerunning the POLYMATH program.

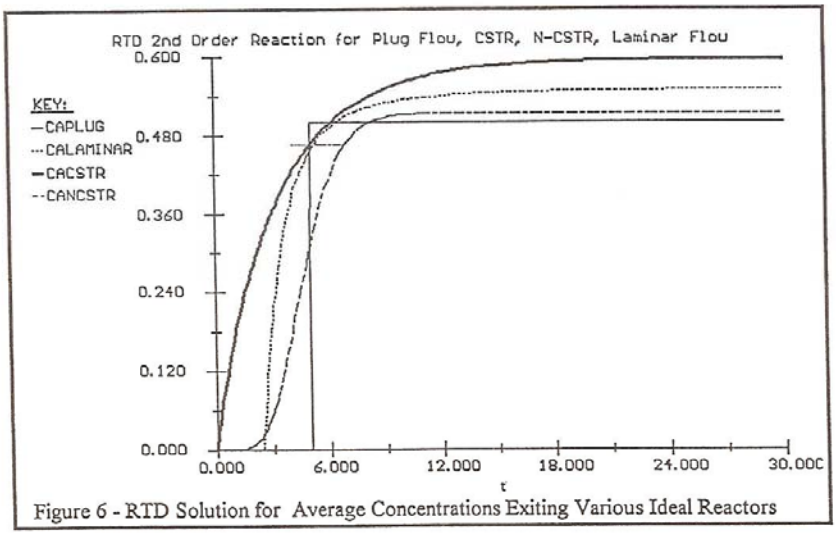

Figure 6 - RTD Solution for Average Concentrations Exiting Various Ideal Reactors

The RTD curves for the various reactors can also be plotted at the request of the user. these are shown in Figure 7 where the characteristics of the various reactors can easily be compared.

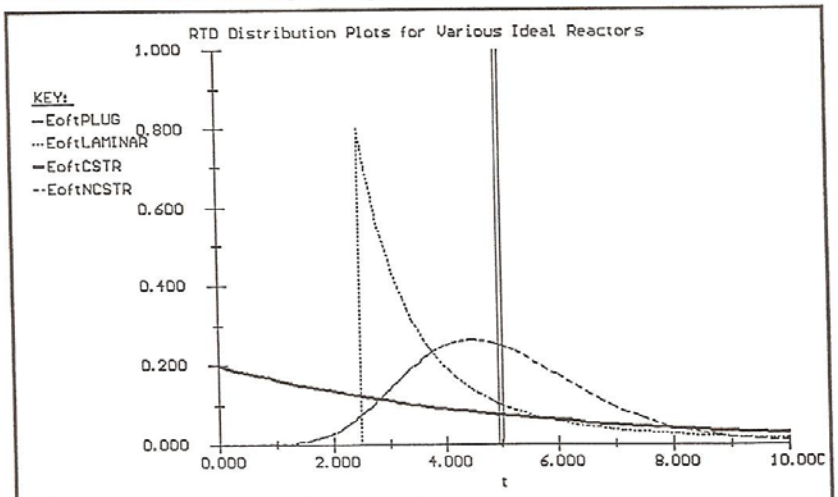

Figure 7 - RTD Functions for Various Ideal Reactors

This example has been for a second order reaction as presented in Equation (3). However, this rate expression can easily be varied in the POLYMATH code so as to consider various types of rate expressions. Thus a single change in one line in the code allows the resulting predicted performance to be calculated from the segregated flow model for a number of RTD's. Extensions to multiple reactions are possible and easily implemented.

In this article we have briefly considered some aspects of nonideal reactor design which illustrate the use of POLYMATH and some convenient new features. Future CACHE Newsletter articles will demonstrate other aspects of this software and its use in Chemical Engineering.

Chemical Engineering Fundamentals in Biological Systems - Multimedia Modules

by Susan M. Montgomery, Kenneth K. Wong, David J. Mooney, Jennifer J. Linderman, Henry Y. Wang, Mark A. Burns, and H. Scott Fogler
University of Michigan

Introduction

Many chemical engineering students are interested in careers involving biological systems. Unfortunately, they seldom see the connections between the chemical engineering fundamentals they learn in the core chemical engineering courses and the biological fields they hope to enter. The goal of this project is to develop multimedia-based educational materials that enable chemical engineering students interested in bioprocesses to make these connections, while providing other students with additional examples of chemical engineering applications. Three modules have been developed so far, and two more are under development, as shown in Table 1. These modules described below have been used in both graduate and undergraduate courses. The results of their evaluation are reported and discussed.

Module Descriptions

Biotechnology's need for visual representation can be realized using multimedia. For example, one can develop animations to demonstrate cell division, giving the students a physical understanding of the biological processes involved. This can be coupled with simulations in which parameters are manipulated, and the animation of the physical process changes according to the changing parameters: a picture of a cell can be shown, then equations relating cell division and, say nutrient concentration can also be shown. Levers might allow students to vary cell concentration, temperature, and/or pH and observe the resulting change in cell division on the screen. Some of these applications were implemented in the following modules.

Chromatography/Adsorption

This tutorial focuses on applications of adsorption to biotechnology. The general equations for adsorption in a column are derived and a chromatography column simulator can be used to explore the effect of various parameters on column performance.

The Introduction to Adsorption section familiarizes users with the qualitative aspects of solute adsorption, desorption, and concentration. The schematic of the column shown in Figure 1 is part of an animation showing solute desorption and concentration.

In the Modeling and Equations section, users learn the mathematical model which governs adsorption. In Figure 2 for example the user has clicked Δz, the length of the unit column section. Red text throughout the module is clickable and will yield the term's definition.

In the Simulator section (Figure 3), the user can specify values for adsorption parameters such as adsorbent diameter, length of column, inlet flow rate, maximum concentration of solute on adsorbent, and the adsorption constant, and learn the relative effects on column performance. The simulation was ported from an earlier PC module for separations courses (Fogler et al. 1992), and is based on one of the author's (MAB) research projects.

The final section of the module is a case study which investigates the use of affinity adsorption to concentrate and purify monoclonal antibodies. The case study of affinity chromatography gives a "real" world example on how protein A is used to bind to the Fc portion of immunoglobulins and thus separate it from other proteins. Throughout the section the user is tested on her knowledge of affinity chromatography by questions which relate material learned earlier in the module to the practical example within the case study.

Receptors

This module reinforces kinetics concepts in the context of a biochemical process. The module includes an introduction to receptor-ligand systems, a quantitative section dealing with kinetics, and case studies from current research at the University of Michigan and elsewhere.

The Introduction (Figure 4) familiarizes users with qualitative issues such as the physiological significance of receptor-ligand binding and how receptor - ligand interactions are analyzed (Lauffenburger and Linderman, 1993). It also introduces and defines biological terms used throughout the module.

The Interaction/Kinetics section addresses the quantitative reaction kinetics issues involved in simple receptor - ligand binding (Figure 5). It is divided into three subsections: transport of ligands, receptor - ligand binding, and post - binding phenomena. Within the binding section the user can access a Visual Basic dynamic simulation of receptor-ligand binding within an Excel spreadsheet. The Simulator (Figure 6) allows the user to change values of process parameters such as ligand concentration, reaction rate constants, total receptors

and initial complexes, and study the resulting effects on receptor - ligand binding.

The Case Studies section (Figure 7) introduces students to specific "real world" applications that involve receptor-ligand interactions within receptor research. This section includes case studies on allergic reactions and tissue engineering. The first case study investigates the role of signal transduction (specifically receptor crosslinking by multivalent ligands) in allergic responses. The case study expands on the kinetics learned earlier to cover the case of crosslinking. The user is then asked conceptual questions to test whether they can recognize the added complexity of the kinetics behind crosslinking. The second case study, on tissue engineering, exposes the user to a different application of receptor-ligand binding by presenting the concept of seeding cells on a matrix. One of the goals of the case study is to ensure that the user has a more holistic view of receptor-ligand interactions than is usually presented in introductory biology books. To achieve this the idea of the ligand being fixed while the cell(and thus the receptor) floats freely is presented in the context of a vascular graft matrix. The user is then asked questions on how to optimize cell seeding for different matrices.

Bio kinetics

This module focuses on bio-kinetics as applied to bioremediation and bacteria profile modification. The module includes a review of bio-kinetics; key requirements for successful bioremediation; and simulations based on ongoing bioremediation research (Figure 8).

The Bio-kinetics section (Figure 9) familiarizes the user with the concept of biological reactions, cells, types of reactors, and products. A quantitative approach to characterize kinetics and reactors is also reviewed for both batch and continuous reactors.

The Bacterial Profile Modification section introduces the user to the use of BPM and its application to oil recovery. In addition the user has the opportunity to use an Excel based simulation of the growth of cells in a batch reactor. Euler's method is used to solve the six differential equations that describe cell growth and substrate utilization (Lappan and Fogler, 1994). The simulator (Figure 10) lets the user vary initial concentrations and kinetic parameters and yields graphs of cell concentration versus time data for the batch reactor.

Bioremediation (Figure 11) is introduced as an application of biological reactions. Requirements for successful bioremediation and different bioremediation techniques such as biostimulation and bioaugmentation are reviewed.

Material Balances in Biological Systems

This module, still under development, will help students in the introductory chemical engineering course understand and practice the application of material balances to biological systems of different dimensions (e.g. cell level to chemical plant level). The module focuses on the use of an algorithm for the solution of material balance problems (Figure 12). Examples will include mass balances on a cheese factory, and a material balance on an artificial kidney.

Oxygen Transport in the Human Body

This module, still under development, will relate concepts taught in mass transfer to biological systems focusing on the role of convection and diffusion in oxygen transportation through the body (Figure 13). The module contains three parts: introduction, quantitative analysis, and case studies. The introduction section familiarizes the student with the concepts of convection and diffusion, and their effects on the transport of oxygen throughout the body. The quantitative analysis section presents the relevant equations of convection and diffusion while demonstrating how they are applied to biological systems. In addition this section presents the Krogh cylinder model, which illustrates how convection and diffusion compete in oxygen transfer through veins. The final section will include two case studies on artificial kidneys and bioreactors, to help the student establish more connections between mass transfer theory and its application to biological systems.

Evaluations

The first three modules described in the previous section were class tested in both the core separations and kinetic classes at the University of Michigan as well as in a new senior-level course, Engineering Fundamentals in Biological Systems, developed as part of this project. Students were asked to complete evaluation forms to ascertain if the modules were helpful in understanding the concepts presented. The results for average time for completion, ease of use (scale of 1 -> 5 where 1 is easy to use) and whether the student would recommend using the module in the future (scale of 1 -> 5 where 5 is strongly agree) are shown in Table 2. The time for the Receptors module does not include running the case studies as they were unavailable at the time. We were very pleased both by the high rankings the module received and the perceived ease of use. The length of time to run the modules was somewhat longer than we hoped for, particularly for the adsorption module.

The following responses were obtained from students in the Open Ended Comments section of the evaluation:

"I plan to use it heavily to prepare for the exam"
"The module was very effective. I had trouble understanding the material in the lecture. After running the module I feel I have a much better grasp of the material."
"The modules need more questions, otherwise it is to easy to just skim through."

"It was nice to have another alternative to reinforce the lecture"

In addition to the above comments the students identified the following as strengths of the modules: the derivation of complex equations, the ability of students to move at their own pace, explorative questions following the simulators, the constant availability of symbol and word definitions, the way the modules integrate varying subjects into a cohesive presentation and present dry subjects in novel ways (movies, graphics, etc.) and the option to get more in-depth information if one was interested.

Some of the concerns reported by the students included: the need for more interaction, long time to complete, the speed at which applications run, getting lost within the module sub menus, and not having enough questions to test material. These concerns will be addressed in updates to the completed modules, and will be avoided in future development.

Future Work

The first three modules (Chromatography/Adsorption, Receptors, and Bio kinetics) have been completed and class tested. They will undergo a second round of class testing during this academic year. Material Balances in Biological Systems and Oxygen Transport in the Human Body, will be tested during the 96-97 school year. The complete set of five biomodules should be available for distribution by CACHE towards the end of the summer of 1997.

References

[1] H.S. Fogler, S.M. Montgomery and R. P. Zipp. "Interactive Computer Modules for Undergraduate Chemical Engineering Instruction," *Computer Applications in Engineering Education* Vol. 1 No. 1, 1992, pp. 11-24.

[2] R.E. Lappan and H.S. Fogler, "*Leuconostoc mesenteroides* Growth Kinetics with Application to Bacterial Profile Modification," *Biotech. and Bioeng.*, Vol. 43, 1994, pp. 865-873.

[3] Lauffenburger, D.A., and J.J. Linderman *Receptors: Models for Binding, Trafficking, and Signaling* . Oxford University Press Inc., New York, New York 1993.

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For additional information please contact:
smontgom@engin.umich.edu

or visit our web page at:
http://www.engin.umich.edu/labs/mel/.

Table 1 - Bio Modules

Module	Course	Status
Chromatography / Adsorption	Separations	Beta Version Ready
Receptors	Kinetics	Beta Version Ready
Bio Kinetics	Kinetics	Beta Version Ready
Material Balances in Biological Systems	Material Balances	Under Development
Oxygen Transport in the Human Body	Mass Transfer	Under Development

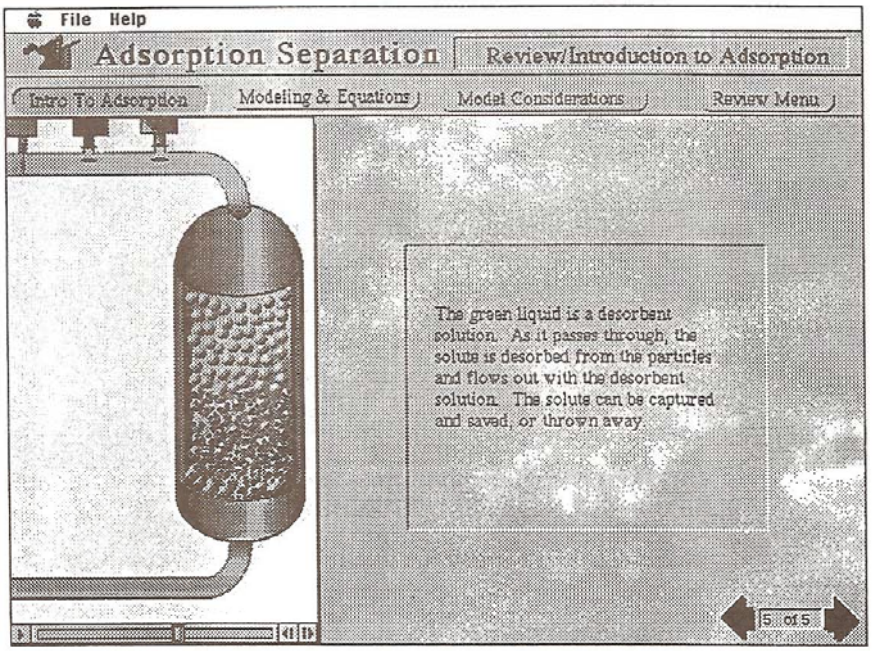

Figure 1. Adsorption Separation module-Introduction

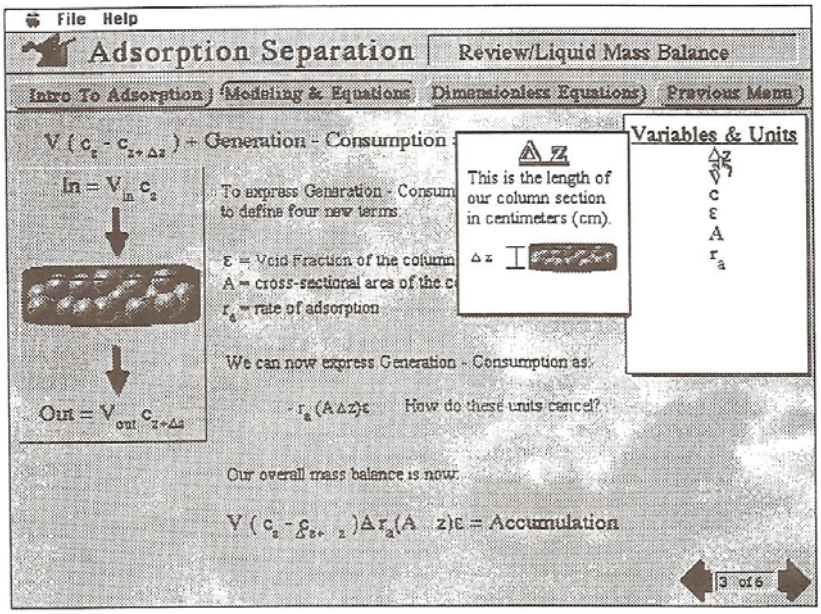

Figure 2. Adsorption Separation module-Modeling Equations

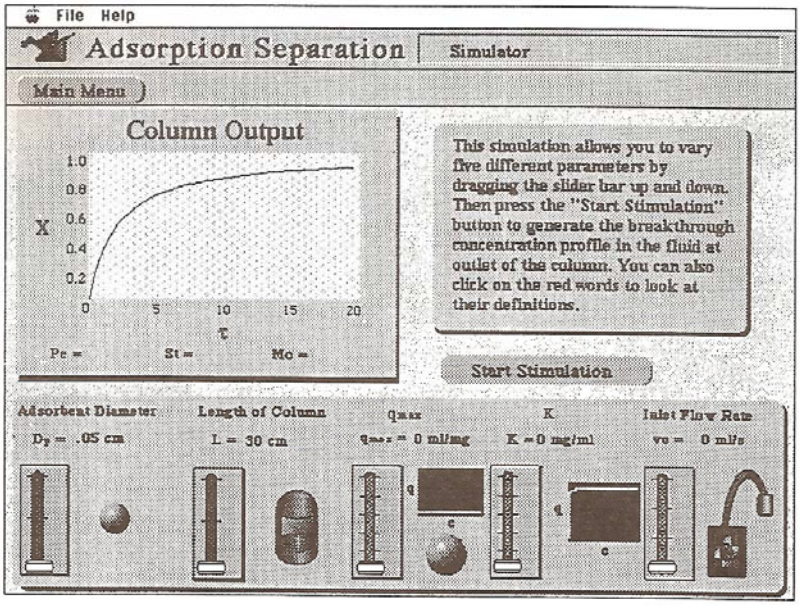

Figure 3. Adsorption Separation module-Simulation

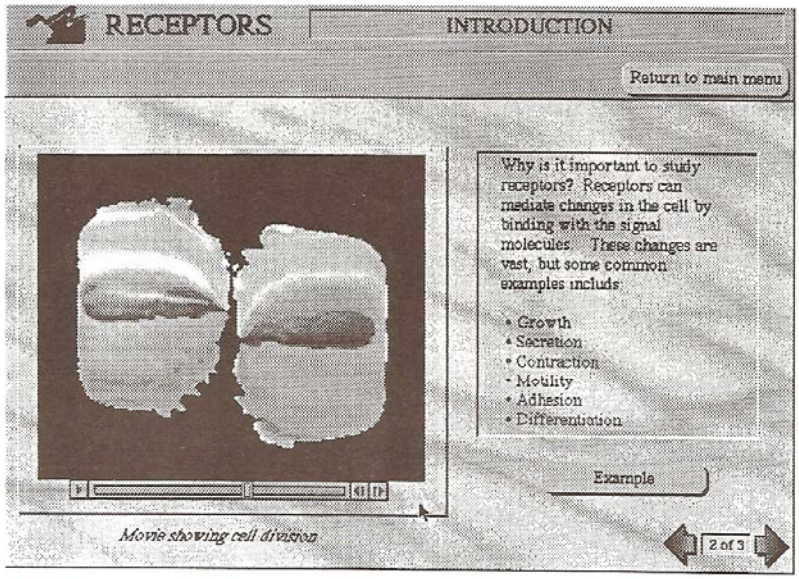

Figure 4. Receptors module-Introduction

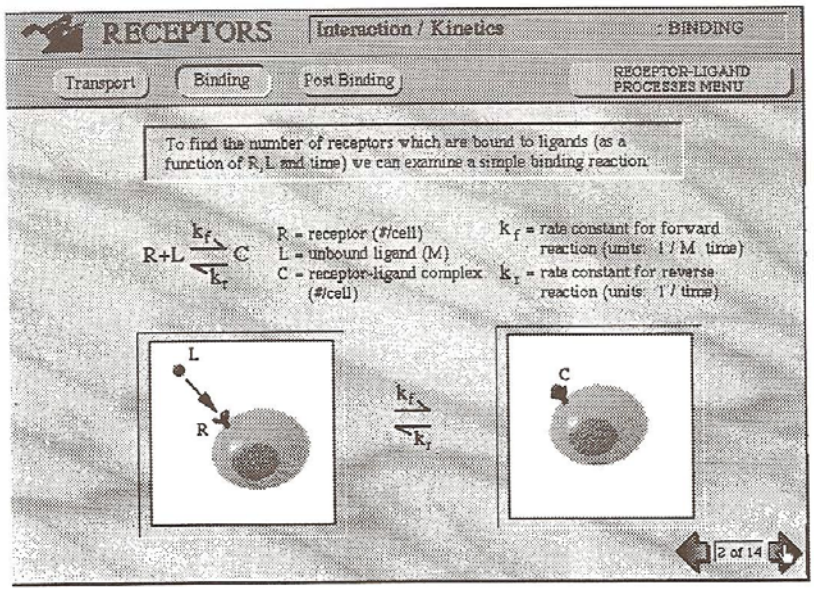

Figure 5. Receptors module-Interaction/Kinetics

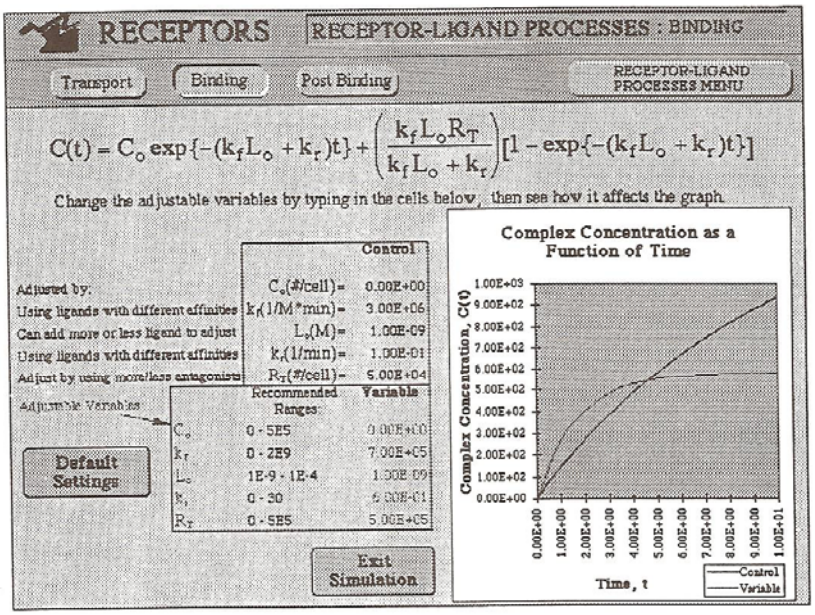

Figure 6. Receptors module-Simulation

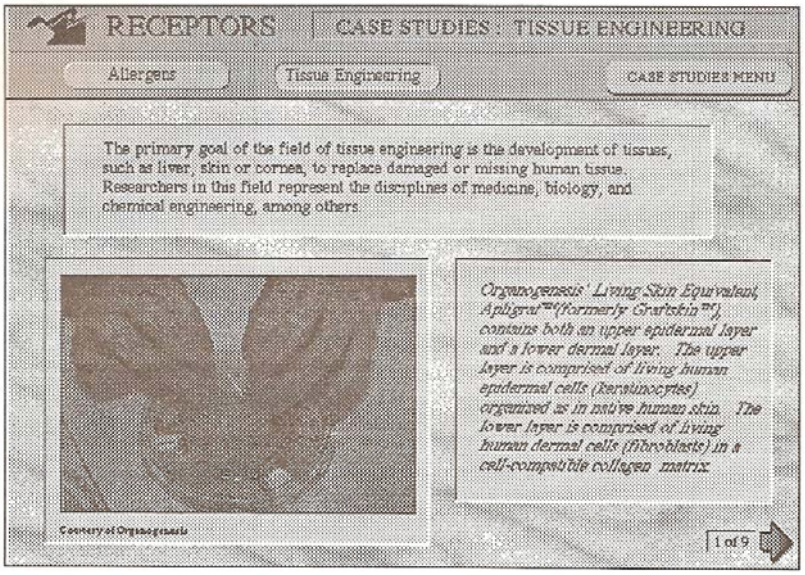

Figure 7. Receptors module-Tissue Engineering Case Study

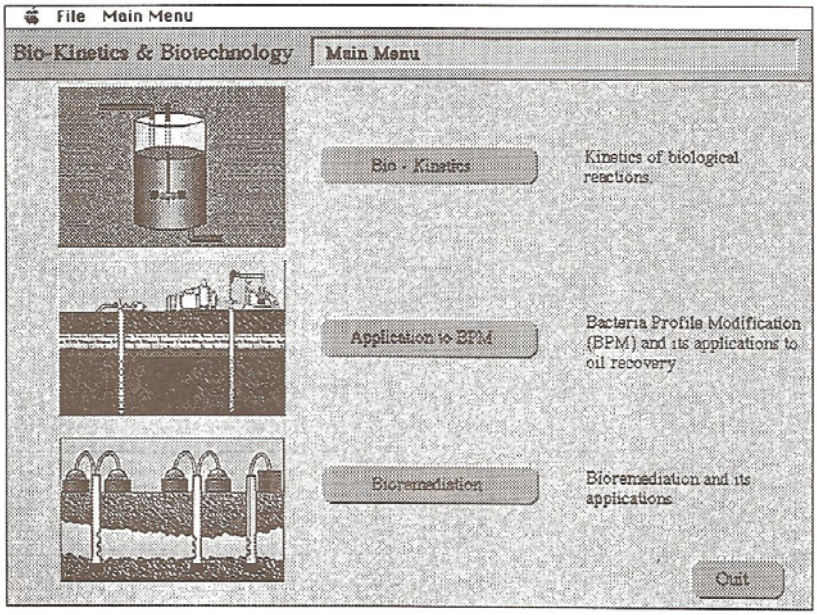

Figure 8. Bio-Kinetics module-Main Menu

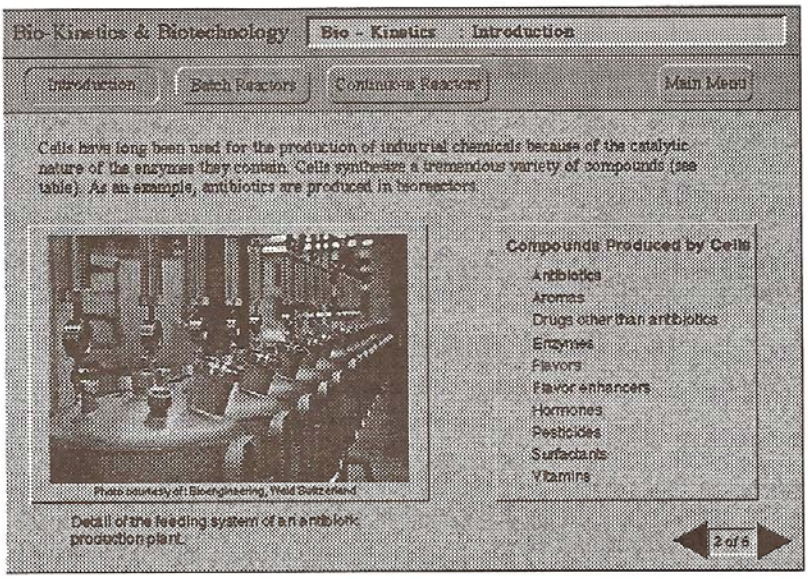

Figure 9. Bio-Kinetics module-Introduction

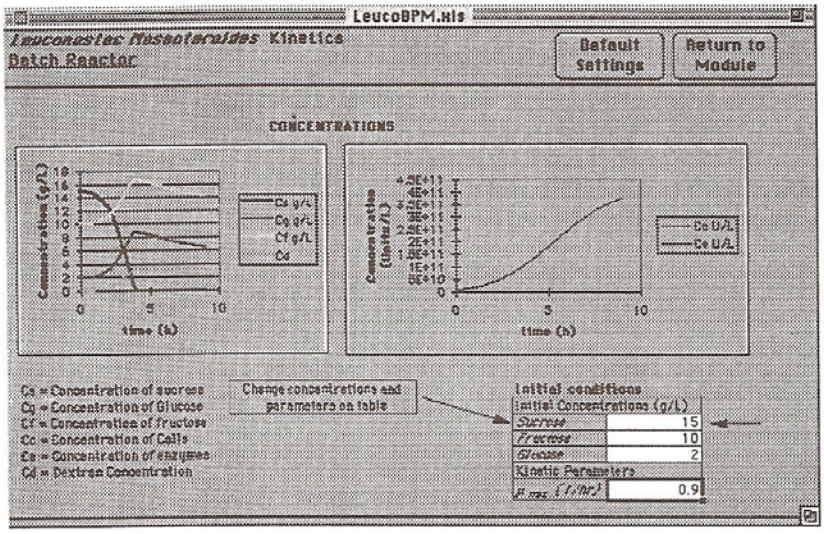

Figure 10. Bio-Kinetics module-Simulation

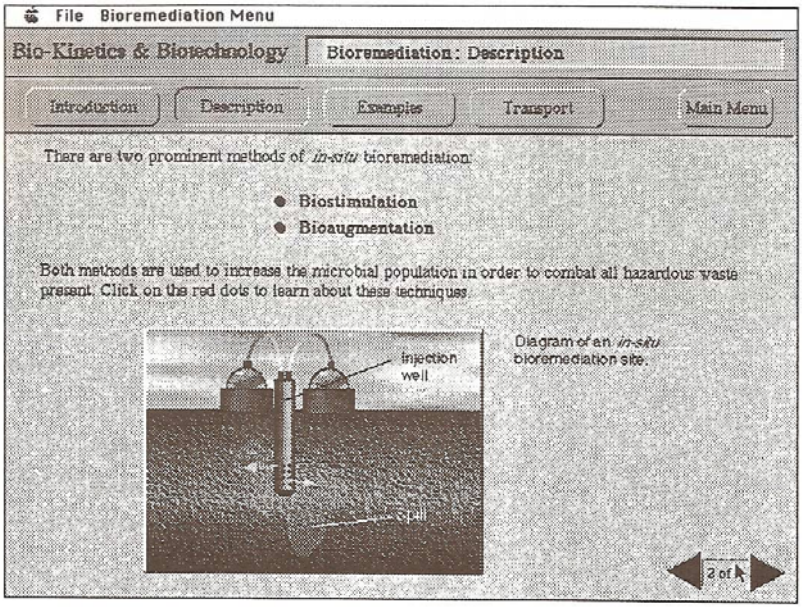

Figure 11. Bio-Kinetics module-Bioremediation

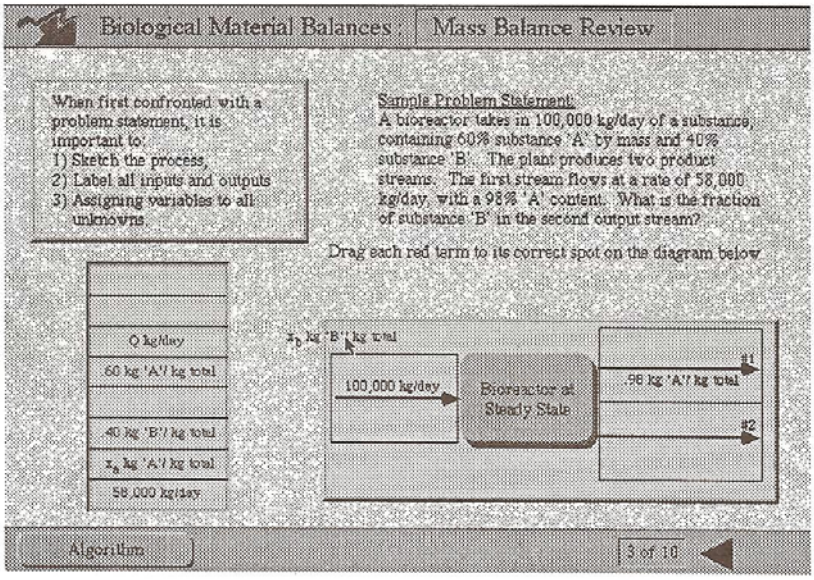

Figure 12. Material Balances in Biological Systems - Algorithm Review

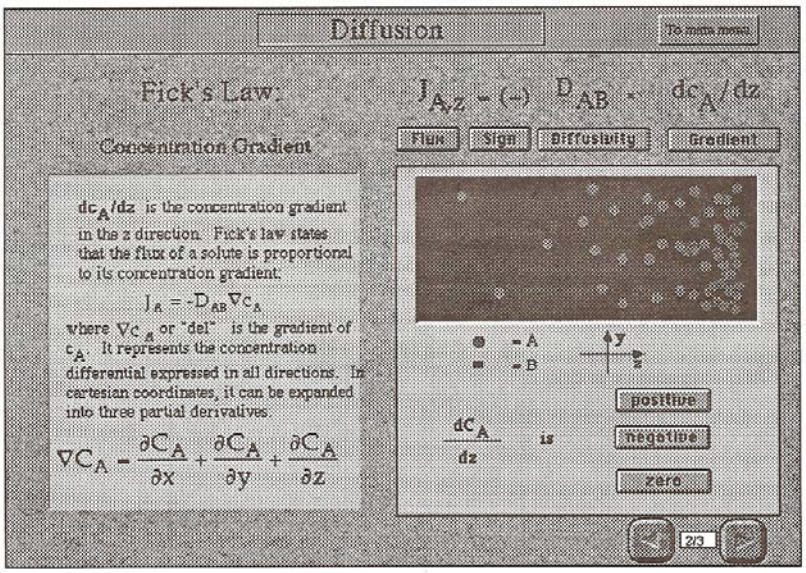

Figure 13. Oxygen Transport in the Human Body - Fick's Law Review

Table 2 - Student Evaluation

	Module		
	Adsorption	Receptors	Biokinetics
No. of testers:	10	17	53
Time (min)	51 ± 17	30 ± 12	46 ± 23
Ease of Use (1-5; 1 is easy to use)	1.3 ± 0.5	1.4 ± 0.6	1.5 ± 0.8
Recommend using (1-5; 5 is strongly agree)	4.5 ± 0.7	4.4 ± 0.6	4.3 ± 0.9

Computational Fluid Dynamics and the Curriculum

by Andrew N. Hrymak, McMaster University

Introduction

- An engineer simulates the flow of air over a new car body looking for vortices in the flow and causes for drag and noise
- A mixing tank is modified after simulation to remove dead zones and a new impeller is added to enhance the turbulence to a particular region
- An injection mold with 64 cavities and a long complex runner system is modeled and the cooling system modified to provide more balanced flow and solidification of the polymer

These are everyday examples of the kinds of problems currently being solved with a new generation of software which solve the momentum, mass and energy equations simultaneously in complex geometries. Computational fluid dynamics (CFD) is the numerical solution of the momentum and continuity equations, but generally includes the transport equations. Complex flow problems are now being routinely solved with the ready availability of computer workstations that are fast and relatively inexpensive, as well as through the advances in commercial CFD codes. The types of problems that are particularly amenable to a CFD package include at least two spatial dimensions and some of the following features:

1. complex geometry
2. turbulence
3. nonlinear material properties, including non-Newtonian behavior
4. free and moving boundaries
5. phase transitions

Software for CFD is important in many fields of chemical engineering, but particularly in materials processing and design of units at a detailed level. There are spectacular successes from the aerodynamics engineering field in using CFD and structural analysis codes to develop the new generation of aircraft. There are still a number of gaps in our understanding of how to model certain types of fluids and fluid flow regimes and limitations in our ability to validate the results of some simulations. The solution of realistic problems requires the combination of a stable set of software tools for problem formulation, mesh generation and robust solution procedures, as well as significant computer power. While CFD technologies have been actively developed and used on "supercomputers" and workstations over the last three decades, the current availability of powerful personal computers now affords a new opportunity to examine this set of technologies in the undergraduate curriculum. This article will explore whether there is an opportunity in the chemical engineering curriculum to systematically develop our students' understanding and abililty to use this new generation of software tools.

Curriculum Issues

One way of looking at the organization of our courses and knowledge is through a classification using length and time scales (Bird, 1993; Krieger, 1996). A generalization of such a structure follows:

Unit operations and process systems (Macroscopic scale): length scales over a metre and time scales of longer than minutes. The fundamental balances are written around units with detail about the inner elements limited to the necessary requirements to calculate product flows and important macroscale parameters. Approximations and correlations are used to provide parameters which link subsystems; e.g., heat and mass transfer coefficients, separation efficiencies. Balances around individual units are linked together to form systems.

Continuum (Microscopic scale): length scales of between a millimetre and a metre and time scales of seconds. The transport equations, or equations of change for conserved quantities, are solved to get detailed values for the state variables within a domain. Important variables include pressure, velocity components, temperature and concentrations. Unidirectional and simplified problems can be solved analytically, more complex systems require asymptotic analysis and other more advanced techniques. Discretized versions of the the transport equations are solved to estimate state variables at predefined positions in space and time. Prescribed relationships are used to define material properties and relationships between fluxes and state variable quanitites; e.g. shear stress and velocity component gradients.

Phase structure: length scales of angstroms to microns and time scales of milliseconds. The continuum equations cannot

be applied directly; structures are formed by tens of thousands of molecules so that molecular dynamics methods are difficult to apply. Phase transitions are important in determining the state of the systems and there is a time evolution of the material properties. Examples include: polymer orientation, foam structure development, crystallization and solidification from a melt. Empirical expressions required for the material properties, flux expressions and length scales over which approximations to the phase state can be made.

Molecular dynamics (Molecular scale): length scales of nanometers and time scales of picoseconds. The equations for the solution force-field models are solved to determine the distribution of the molecular entities. Requires approximations for the intermolecular forces. If enough molecules can be included within a simulation over a long enough period of time, then quantities such as diffusivity, viscosity and thermal conductivity can be estimated. Rearrangements of molecular structures can be observed in simulations and length scales compared to experimental measurements.

Process Systems Analysis

The undergraduate curriculum is largely devoted to the macroscopic scale. The layering of courses builds on a unit operations approach to develop a working knowledge of process systems engineering.

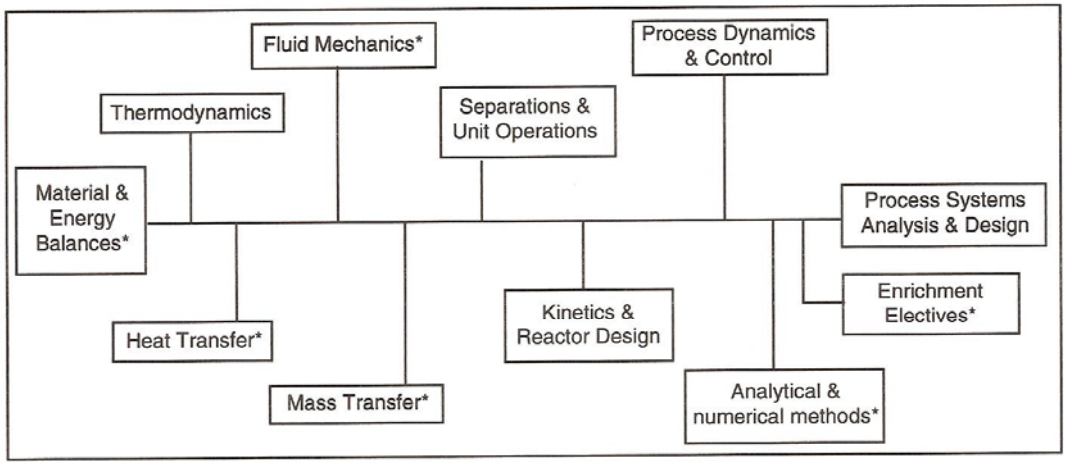

Figure 1. Simplified view of the Chemical Engineering Undergraduate Curriculum.

The curriculum builds on the basic concepts introduced in the material and energy balance course leading to a unit operations understanding and finally to the development of process analysis and design (synthesis and optimization as well in some curricula). The introduction of computer tools parallels the development of the complexity of problems in the courses. Computer software tools include:

1. spreadsheets,
2. engineering and symbolic calculation programs (e.g. Polymath, CACHE Corp.; Mathcad, Mathsoft Inc.; Maple, Waterloo Maple Software; and Matlab, Mathworks Inc.),
3. specialty flowsheet tools (e.g. ChemSep, CACHE Corp.) and
4. commercial process flowsheeting software (e.g. AspenPlus, Aspen Technology; Hysys, Hyprotech; and ProII, Simulation Sciences).

Unit modeling is conveniently done with the first two classes of software tools where the student can implement (or use existing code for) the underlying fundamental balances, calculations for equipment and material parameters and other necessary engineering calculations. Numerical methods courses provide the necessary knowledge for the solution of these models which contain linear and nonlinear, algebraic and ordinary differential equation sets. However, specialty and commercial flowsheet simulators also allow access to a thermodynamic and physical properties database, convenient linking of process units, switching between types of unit models, dynamic simulation and steady-state optimization. The jump between the types of calculations done by the students on the first two classes of tools and the latter two classes is huge. The algorithms used to calculate certain types of units (e.g. inside-out methods for distillation columns) are not normally covered in detail in the undergraduate curriculum and implementation

would be a formidable exercise. Students use the more advanced tools effectively in their senior design courses because the key concepts and input variables are usually consistent between different modeling levels. The students do not particularly have to worry about the detailed implementation of the models within a flowsheet simulator, but they do have to learn and practice the skills of properly posing problems.

Transport Phenomena

Two or more spatial dimensions, transient effects, nonlinear physical properties and convective model components are parts of more complex and realistic problem specifications found in problems at the microscale. Approximations to the problem can be solved using advanced applied mathematics to provide analytic solutions (Bird, Stewart, Lightfoot, 1960; Finlayson, 1980; Denn, 1980; Leal, 1992).

General problems require the solution of the conservation equations for mass, momentum and energy. An approximate solution to the state variables is defined at discrete points, or nodes, within the domain. The discretizatized set of equations replaces the PDE set by an algebraic or differential equation set. There are a number of common methods used to convert the PDE set to algebraic equations: finite differences, finite volumes, finite elements and collocation methods. In the *finite difference* method the derivatives of the state variables are approximated using Taylor Series expansions. *Finite or control volume* methods (Patankar, 1980) satisfy the integral form of the conservation equations. Variations on the finite volume methods depend on how the control volume is chosen around the nodal points and the manner in which gradient terms are approximated using neighboring nodes and their respective control volumes. *Finite element* methods use a locally defined polynomial for each state variable over a small region within the domain with the values of the state variables at defined nodes such that the residual is forced to zero through a weighted integral of the residual error. Local polynomial approximations with the specification that the residual error be zero at specified sampling points is called *collocation* (Finlayson, 1980). The discretized solution methods require a network of nodes, which will define the points at which the state variables will be determined. The generation of this network is called *gridding* or *meshing* the flow domain. The basic steps in the solution procedure are: choose the conservation equations and terms within the equations appropriate to the problem, divide the domain into an appropriate set of nodes and subdomains/elements, assemble the discretized forms of the PDEs as (non)linear algebraic equations and solve the equation set. Sample reference textbooks for each of the methods as applied to CFD include: Anderson et al. (1984) for finite differences, Baker (1983) and Dhatt and Touzot (1984) for finite elements and Patankar (1980) for control volumes. Minkowycz et al. (1988) and Fletcher (1988) provide chapters dedicated to the use of different numerical schemes common in CFD applications.

Bridging the Two Approaches

There are a number of parallels between CFD and process flowsheeting or systems analysis as currently taught in the curriculum

Process Flowsheeting
- Fundamental material and energy balances
- Linking of balances to take account of staged, distributed parameter and linked unit processes
- Linkage of unit models through process topology
- Solution of nonlinear algebraic equations by taking ad vantage of structure or equation sparsity

Computational Fluid Dynamics
- Conservation equations for momentum, energy and mass
- Formulation of the discrete form of the conservation equations using finite volumes, finite elements with a weighted residual
- Linkage of local approximations through the use of a mesh topology
- Solution of nonlinear algebraic equations by taking advantage of structure or equation sparsity.

If we take a look at the curriculum from another viewpoint, then one can see a "transport based approach" that can use CFD software currently available. In Figure 1, the subject areas with a * in the box could be coupled together to form a stream where the continuum or microscopic scale of analysis could be pursued to a design project involving the numerical solution of coupled transport phenomena. An example of book that promotes this design approach is that of Baird and Collias (1995) for polymer processing. Idealized flow problems or approximations to more complicated problems can be solved with tools such as spreadsheets, symbolic solvers and engineering software tools. More complex problems coupling different types of conserved quanitites in complex geometries require CFD software tools.

Dr. Philip E. Wood and I have offered an introductory graduate course in computational fluid dynamics for a number of years with students from chemical, mechanical, civil and materials engineering. The course outline is as follows:

- Governing momentum and energy equations, Navier-Stokes equations, conservative and non-conservative forms, turbulence models, wall functions, boundary conditions
- Control volume method, gridding (staggered and non-staggered), discretization

- Solution of large sets of algebraic equations, direct methods, iterative methods, tridiagonal forms, Stone's implicit method, alternating direction implicit method and relaxation
- Convective terms, upwinding
- Pressure-velocity coupling, SIMPLE and variants
- Boundary fitted coordinates, covariant and contravariant velocities, generalized coordinates, metric tensors, solution methods, velocity interpolation methods
- TEACH code, FLUENT -BFC code

Students who have taken this CFD course have had a background which ranged from a first fluid mechanics course, to a course using a text such as *Transport Phenomena* (Bird, Stewart and Lightfoot, 1960), to having advanced fluid mechanics and heat transfer courses. Our course covers the material from the point of view of someone who would like to write a CFD code, as well as someone who will use a commercial CFD code. In recent offerings, we have changed from having students write or modify existing source code to using commercial code to solve more realistic industrial problems. We therefore make the same leap that is common in the current unit operations based curriculum; i.e. derive, analyze, and implement relatively simple problem solutions to provide the knowledge framework, discuss the references to more advanced implementation aspects (e.g. iterative solvers and advanced meshing techniques) and then move to commercial codes. The practical problems we choose as projects for the students have complex geometries, but usually either simple constitutive relationships or turbulence models. In essence, the course synthesizes the key elements of the transport courses (without the analytical solutions possible for simplified problems or approximations to more complicated cases) and then moves quickly to the "design" elements by using the CFD tool as a means of calculating the velocities and pressures in realistic flow configurations. This course is designed to be an integrating course for fluid mechanics, selected numerical methods and the use of a CFD software tool. If the course were offered with the scope limited to laminar Newtonian flow problems, in complex geometries, such a course would be similar to undergraduate courses offered in mechanical engineering and civil engineering departments for the solution of finite element problems for plates, shells and beams.

The most time consuming aspect from a user's point of view in using current CFD packages is the time required to mesh the flow domain to provide the coordinates for the points (nodes) at which the state variables will be calculated. A rough guide is that 80% of the user's time will be spent in preparing the mesh. If the mesh is too coarse, then the solution will be inaccurate and in some cases, the problem will fail to converge. If the mesh is too dense, then the solution times and computer resource requirements (memory, hard disk) become too intense for solution on modest computing facilities. The most important advance in current CFD technology for the user (and student) is the graphic interface that has been developed to mesh and post-process the results. Data input and output with separate post-processing was done for many years, but it was time-consuming and expensive. The current methodology combines the pre- and post-processing (i.e. meshing and visualization) steps as part of the solution procedure which is critical for determining the causes of solution problems. From a teaching perspective, it aids the student if the problem geometries are chosen so that a reasonable amount of time is spent on the meshing. Alternatives are to provide mesh templates for problems which can be modified. The whole area of how meshing is done is rapidly changing, especially with new automated meshing procedures (e.g. Blacker and Stephenson, 1990).

Codes Available

The following is not all inclusive but provides examples of commercial codes that the author has used in teaching and research. FIDAP (Fluid Dynamics International, Evanston, IL), NEKTON and FLUENT (Fluent Inc., Lebanon, NH) are examples of codes that solve a wide variety of CFD problems both in gas and liquid flows. FIDAP and FLUENT have turbulence models included within their libraries. They have some capability for non-Newtonian flows, but not viscoelastic materials. All three codes can solve 2-D and 3-D problems, with moving boundaries and free surfaces, depending on the geometry. NEKTON has been especially tailored for coating flows which are marked by free surfaces and complex geometries. POLYCAD (Polydynamics, Hamilton, Ontario) is currently available in a 2-D version and solves flows common in the polymer processing industries. FIDAP and POLYCAD are based on the finite element method, FLUENT is based on the finite volume method and NEKTON uses the spectral finite element method. For a student, the differences in underlying methodology are important in assessing the strengths and limitations of the code for a particular problem class and the terminology and best structure for the mesh.

An example of a specialized class of CFD simulators is C-MOLD (AC-Technology, Ithaca, NY) which is used to model injection molding of thermoplastics (with additions to the code for reactive molding). With C-MOLD, a user is able to model the melt flow within the flow runners and cavities, and then the subsequent cooling of the material. This class of program is widely used in the injection molding and related industries to help design the molds, cooling lines and determine the cycle times and economics for the process. With the stress on quality and continuous improvement in the materials processing industries, such packages are becoming widely used in industry.

The annual *CEP Software Directory* provides a convenient listing of many of the major general and specialized (industry-specific) CFD codes. Another source of information that I found interesting were the web pages of the major

computer vendors who list in their applications directories many of the major software vendors (see http://www.cray.com/ and http://www.sgi.com/ for sample lists of CFD software). Some of the packages are available only on certain computer platforms. A number of the CFD packages are now available on 32-bit personal computer class processors.

Application Areas

There are many examples of flows studies in industry. It is particularly useful for the student to use data for velocity and pressure from an experimental study in the literature and then develop the CFD solution for the same flow field. The ability to compare experimental data to the calculated quantities provides valuable experience when the student then has to develop CFD solutions for new geometries where such validating data may not be available.

Examples of application areas include the following.

Classic laminar flows:

- flow in a pipe
- parallel flow between two plates
- flow past a circular cylinder
- flow in a converging channel
- fluid flow in a square duct with a 90 degree bend
- flow over a backward facing step
- Stokes flow in a wedge

Fluid flow and heat transfer:

- evaporating water spray in a two-dimensional duct
- natural convection in a cavity
- airflow over multiple steps in a channel
- flow past a heated obstacle
- heat transfer in a fuel-rod assembly
- flow and heat transfer in an in-line tube bundle

Turbulent flows:

- turbulent flow over a backward-facing step
- turbulent flow in a pipe

High speed flows:

- transonic flow in a converging/diverging nozzle
- supersonic flow over an obstacle in a channel

Flows in mixing devices:

- fluid flow and heat transfer in a mixing elbow
- particle suspension in a mixing tank
- baffled mixing tank
- jet impingement in a narrow axi-symmetric channel

Free and moving surfaces:

- spin-up of a liquid in a vessel
- development of a drop
- double roll coater

Phase change in materials processing:

- phase change in continuous casting
- thermocapillary convection
- crystal growth from a melt
- conduction melting
- natural convection in steady solidification

Polymer processing:

- non-Newtonian flow in a channel
- die-swell
- slot coater
- injection molding
- profile extrusion die

Electronic materials:

- chemical vapor deposition
- Bridgman technique for crystal growth

Flow, heat transfer and reaction:

- chemical mixing and gaseous combustion
- liquid fuel combustion
- pulverized coal combustion

Porous media flows:

- seepage flow
- flow through a filter

An Invitation

The use of process flowsheeting tools in the curriculum over the last few decades has progressed from implementation of a few unit models through student coding, through executive programs such as GMACS and on to the introduction of FLOWTRAN into the curriculum through the efforts of CACHE Corp. and Monsanto Corp. There are now a number of flowsheet simulators used in virtually every chemical engineering undergraduate program. These programs are the same as those used in industrial practice and provide a bridge between the chemical engineering curriculum and the problems students will face in industry. Evolution in the teaching of process analysis and design facilitated the use of commercial process flowsheeting packages in the curriculum for case studies that would have required a lot of efffort in custom coding without the availability of the commercial process flowsheet simulators.

The situation for CFD now is in some ways similar to that of process flowsheeting and analysis. The undergraduate curriculum has the basis for development of the transport phenomena approach further through enrichment courses or design studies. There is a need for more advanced software so that more realistic problems can be undertaken. CFD courses and case study projects using commercial software tools have been proven at the graduate level. Is there an opportunity in the undergraduate curriculum for a different view of design and analysis?

I would like to invite readers to contact me and share information about courses given at the graduate or undergraduate levels using the tools I have discussed in this article. In a future issue of CACHE News I will summarize your responses, level of interest in these tools and provide a synopsis of the needs that still remain.

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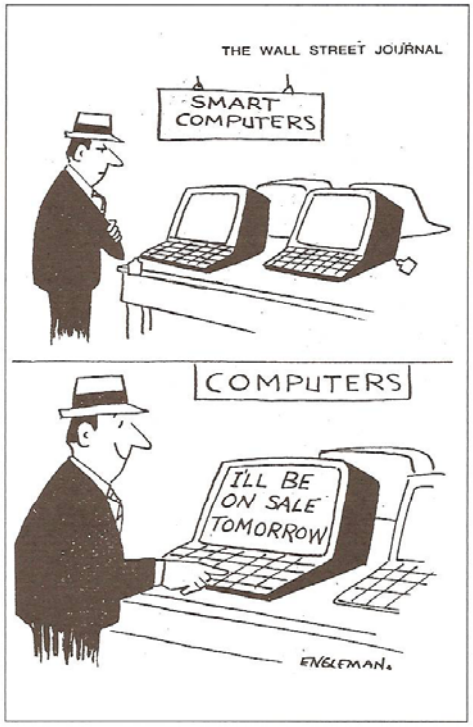
Address of the author:

Andrew Hrymak
Department of Chemical Engineering
McMaster University
Hamilton, Ontario, Canada L8S 4L7
Tel: (905) 525-9140 Ext. 23136
Fax: (905) 521-1350
E-mail: hrymak@mcmaster.ca



Controller Design Made Easy with Digest™ Version 3

By Douglas Cooper and Carlos Velazquez-Figueroa
University of Connecticut

Introduction

Digest, a companion product to Picles ™, is DOS compatible software now being used in process control courses around the world. Digest is an easy-to-use tool for modeling process dynamics and for designing and tuning controllers. Digest is not just an educational "toy." In fact, the package is currently being used by about a dozen companies for the dynamic modeling and controller tuning of real operating processes.

In the process control course at the University of Connecticut, students are first introduced to the concept of modeling process dynamics by way of graphical procedures applied to open loop step test data. Through this graphical analysis, students develop an intuitive feel for the basic model parameters of steady state process gain K_p, overall time constant, τ_p, and apparent dead time, θ_p.

They then learn to use these model parameters in tuning correlations including ITAE (integral time weighted absolute error), IAE (integral absolute error) and IMC (internal model control). These correlations yield initial estimates for the adjustable tuning parameters required to implement P-Only, PI and PID controllers.

After a few weeks, the students are taught how to employ a software package for the modeling task. Possible choices range from Excel to Polymath to Matlab. These fine packages are extremely powerful and offer the potential for broad use outside of process control applications. At UConn, however, we primarily use Digest for dynamic modeling and for computing initial controller tuning values.

Whether the process is found in Picles, another software package, the senior lab, an industrial pilot plant or an actual production facility, consider that designing a controller entails the following steps:

1. The manipulated variable is stepped, pulsed or otherwise perturbed, usually in open loop (manual mode),
2. The manipulated and measured variable data are recorded as the process responds to the input change,
3. A low order linear dynamic model is fit to this manipulated-to-measured variable data,
4. The resulting linear dynamic model parameters are used in a correlation to obtain initial estimates of the controller tuning parameters,
5. The tuning parameters are entered into the controller, the controller is put in automatic (the loop is closed) and controller performance is evaluated in tracking set points and rejecting disturbances,
6. Final tuning is performed on-line and by trial and error until desired controller performance is obtained.

Digest is designed to quickly and easily perform steps 3 and 4 above. The process data must be a text file with columns of data separated by tabs, commas or spaces. Simple commands are used to mark the columns which contain the manipulated input variable data, the measured output variable data and the time data. The linear models available in the Digest model library include:

1. First order,
2. First order plus dead time,
3. First order with integrator,
4. First order with integrator and dead time,
5. Second order,
6. Second order plus dead time,
7. Second order with lead element, and
8. Second order with lead element and dead time.

The selected model is fit to the data by minimizing the sum of the squared errors (SSE) between the actual measured response and the predicted model response when using the actual manipulated variable process data contained in the file.

$$SSE = \sum_{i=1}^{N} [\text{Measured Data}_i - \text{Model Data}_i]^2$$

In computing the SSE, Digest assumes that the process is at steady state before the dynamic event occurs and that the first data point in the file is a good median value of that initial steady state. If these assumptions are not true, the accuracy of the model fit will be reduced.

Once the model has been fit to the data, Digest automatically uses the model parameters to compute initial tuning estimates for the range of PID controllers. If a control computer is so capable, the dynamic model from Digest can be used in those advanced controllers which employ a dynamic model as part of the architecture. These range from a simple Smith predictor up through the full model predictive control (MPC) algorithms.

Digest can also be used to design feed forward elements. For such a design, it is the disturbance variable which should be stepped, pulsed or otherwise perturbed.

After reading the data into Digest, simply select the disturbance data column as the manipulated input variable. The dynamic model fit by Digest will then describe the disturbance-to-measured variable dynamics in a form useful for feed forward controller design.

This Case Study

The case study presented here demonstrates the use and capabilities of Digest when applied to a control experiment from UConn's senior lab. In this case study, Digest is used to fit a low order linear dynamic model to process data collected from a steam heated tank process. Digest uses these model parameters to compute initial tuning parameter estimates for a PI controller first for set point tracking and then for disturbance rejection. The experiment is completed by returning to the steam heated tank, entering the tuning parameter values from Digest into a Foxboro 760 controller and evaluating closed loop performance.

Experimental Apparatus

As shown in Figure 1, the experimental apparatus is a steam heated tank process. Cold water flows into the tank, is heated by a steam coil and exits through an overflow weir. This design results in a constant water volume in the tank. A motorized impeller is used to ensure the water in the tank remains well-mixed.

The measured variable for this experiment is the temperature of the water in the tank. It is measured by a J-type thermocouple and the signal is transmitted to the Foxboro 760 controller, which is programmed to convert the thermocouple electrical signal directly into a temperature reading in degrees Fahrenheit. To introduce additional lag into the temperature measurement and make tight control more challenging, the thermocouple tip is shielded with a small length of flexible plastic tubing.

The manipulated variable is the flow rate of steam through the coil. The steam condenses in the tank coil and passes to a drain. Steam flow rate is regulated by a Foxboro pneumatic control valve connected to the controller. The controller's 4-20 mA output signal passes through a current to pneumatic (I/P) transducer to produce the 3-15 psig signal required to actuate the air-to-open valve. In manual mode, valve position can be adjusted from the controller's key pad.

The disturbance variable for this experiment is the flow rate of cold water being fed to the tank. It is measured with a rotameter and is adjusted with a hand valve. A three pen strip chart continually records the manipulated steam flow rate, the measured tank temperature and the user specified set point.

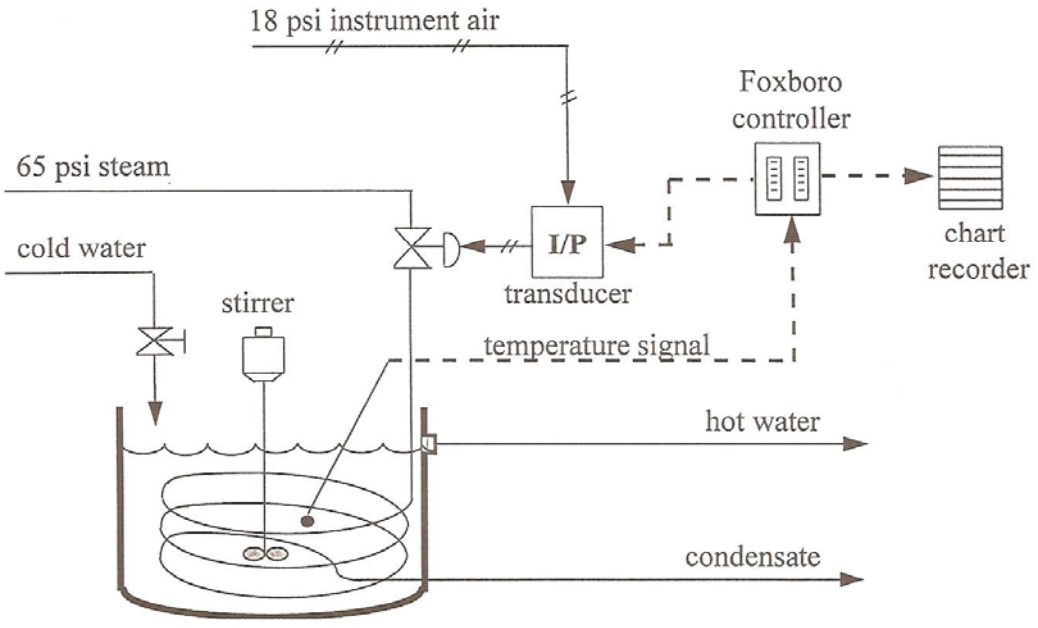


Figure 1. Schematic of steam-heated tank experiment

Open Loop Step Test

Following the procedure detailed earlier, the first step for controller design is to perturb the manipulated variable and record the measured variable as the process responds. The steam-heated tank process, like most found in the chemical process industries, has a nonlinear dynamic character. That is, the steady state process gain, overall time constant and apparent dead time differ as operating level changes. As a result, it is good practice to generate the dynamic data at the level of operation expected when under closed loop control.

In this study, the design measured variable value, tank temperature, is chosen as 90°F. The design disturbance variable value, cold water feed rate, is chosen as 3 gpm (gallons per minute). Thus, it is desired to collect measured variable data which brackets 90°F while the disturbance variable is at its design value of 3 gpm. Although Digest can analyze virtually any manipulated variable sequence, the experiment presented here employs a simple step test.

Thus, using the front key panel of the Foxboro controller while in manual mode, the controller output (the manipulated variable from the controller's view point) is set at 10%. As shown in Figure 2, the measured temperature steadies at about 81°F for this valve position. Then, the controller output is stepped to 25% and the measured temperature responds, ultimately reaching a value of about 100°F.

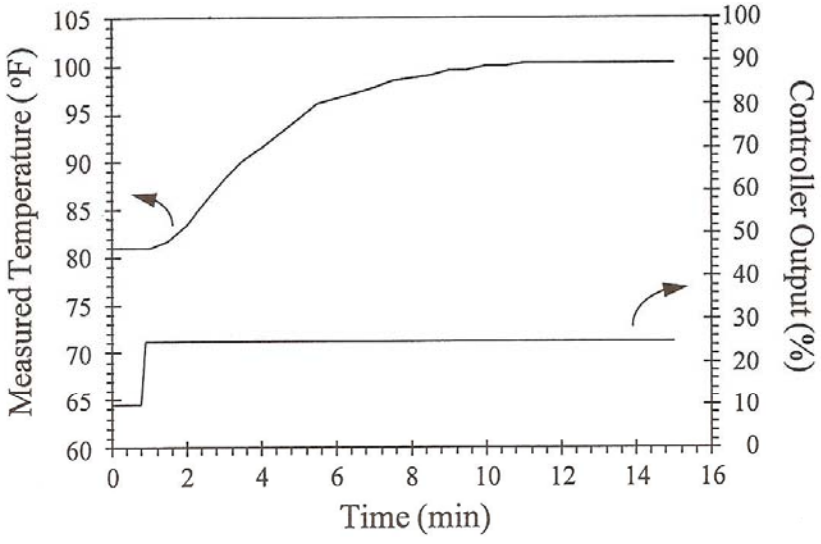


Figure 2. Open loop step test on steam-heated tank

Figure 2 is a computer plot of the actual strip chart, a scan of which is shown in Figure 3. To convert the strip chart into the computer plot, the students must be aware that two different scales are used. The controller output (manipulated variable) ranges from 0-100% across the entire span of the chart as indicated by the scale appended to the right of the chart image. For the measured temperature, the span is 50-200°F, as indicated to the left of the chart image. Time is read based on the speed of recording of the strip chart, which for this experiment corresponded to 3/4" per minute.

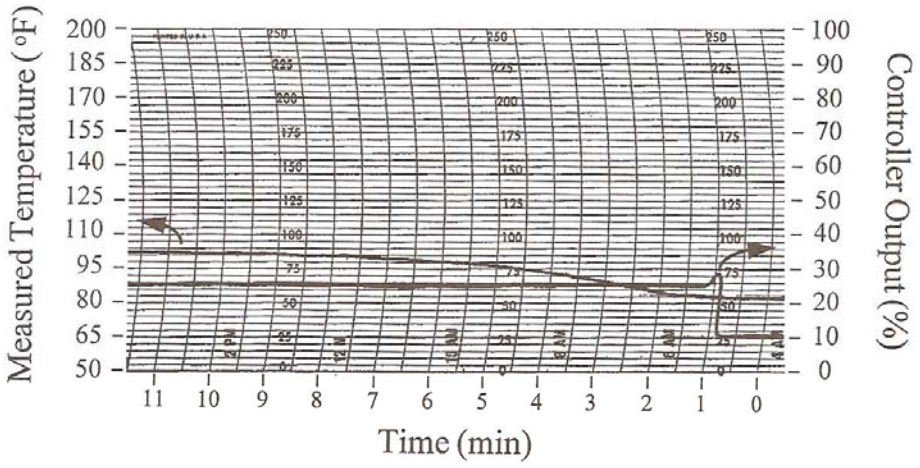


Figure 3. Actual strip chart from open loop test on steam-heated

Dynamic Modeling Using Digest

After translating the strip chart data into text file form, the data can be imported directly into Digest. Once inside Digest, the manipulated input data and the measured output data columns are labeled with a few key strokes.

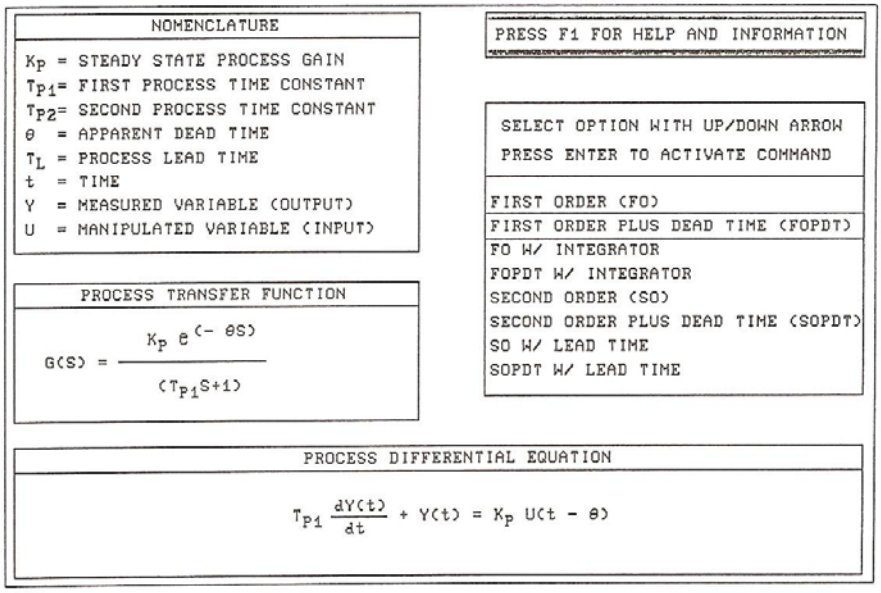


Figure 4. FOPDT model is selected from Digest's library of models

Next, the linear model form desired by the user must be selected from the library of models. For this study, a first order plus dead time (FOPDT) model is selected as shown in Figure 4. For the convenience of the user, Digest displays both the time domain differential equation and the Laplace domain transfer function forms of the model under consideration.

After a few more key strokes, Digest fits the FOPDT model to the data and as shown in Figure 5 for this experiment, displays the result.

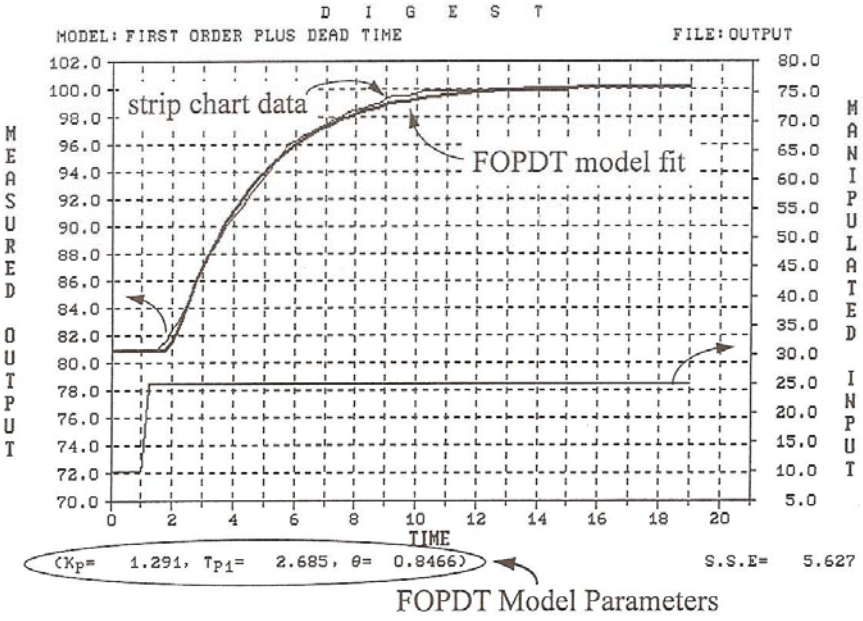


Figure 5. FOPDT fit by Digest to the experimental data

As shown at the bottom of Figure 5, the dynamic behavior of the steam heated tank process can be described by a FOPDT model with parameters:

$$K_p = 1.3 \frac{^\circ F}{\%}$$

$$\tau_p = 2.7 \text{ min}$$

$$\theta_p = 0.8 \text{ min}$$

Controller Tuning

As shown in Figure 6, Digest offers six correlations for tuning a PI controller based on FOPDT model parameters. In this experiment we consider set point tracking and disturbance rejection as two separate designs. In practice, however, a single set of tuning parameters must be determined for any application.

For the set point tracking case, the IMC correlation is chosen, though one of the other relations is arguably as valid for computing initial tuning estimates. The heuristic programmed into Digest for determining τ_C, the closed loop time constant for the IMC correlation, is $0.1\tau_p$ or $0.8\theta_p$, which ever is larger. If a different closed loop time constant value is preferred, it can be changed on the menu and new PI tuning values will automatically be computed.

For the disturbance rejection case, the ITAE for Disturbance Changes correlation is employed. This choice make sense because the correlation was designed with disturbance rejection in mind. The IAE for Disturbance Changes correlation is another candidate which might be considered.

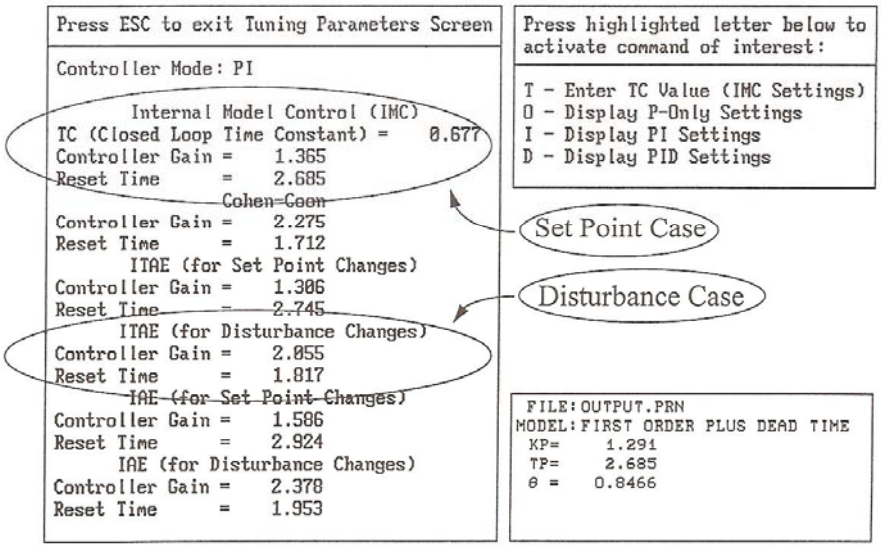


Figure 6. Tuning parameters calculated by Digest

Digest computes controller gain K_C, for the proportional term of a PID controller. The Foxboro 760, however, requires entry of the alternative proportional band, PB, on its key pad menu. Since the controller for this application is programmed such that as the measured temperature varies from 0-100% of its total range (50-200°F), the controller output varies from 0-100% of its range (4-20 mA), then the proportional band required for this experiment is computed from controller gain by the relation:

$$PB = \frac{100}{K_C}$$

Set Point Tracking Case

Based on Figure 6, the IMC tuned PI controller proportional band, PB, and reset time, τ_I, computed by Digest for the set point case are:

$$PB = \frac{100}{K_C} = \frac{100}{1.37} = 73\ \frac{°F}{\%}$$

$$\tau_I = 2.7 \text{ min}$$

Note that, as shown in Figure 6, Digest employs the heuristic that $\tau_C = 0.8\,\theta_p$ when computing the controller gain for this case. Figure 7 shows the set point tracking capability of the controller. The data was originally collected on the strip chart recorder and converted to Figure 6.

To test set point tracking performance, the set point was initially set to 80 °F, and the temperature was permitted to steady. The set point was then stopped to 100°F, thus bracketing the design set point of 90°F. As shown, the controller produces a 10% overshoot and complete settling in one oscillation of the measured temperature. The disturbance flow rate (not shown) was constant at 3 gpm during the experiment.

Disturbance Rejection Case

Based on Figure 6, the ITAE tuned proportional band, PB, and reset time τ_I, computed by Digest for the disturbance rejection case are:

$$PB = \frac{100}{K_C} = \frac{100}{2.06} = 49\ \frac{°F}{\%}$$

$$\tau_I = 1.8 \text{ min}$$

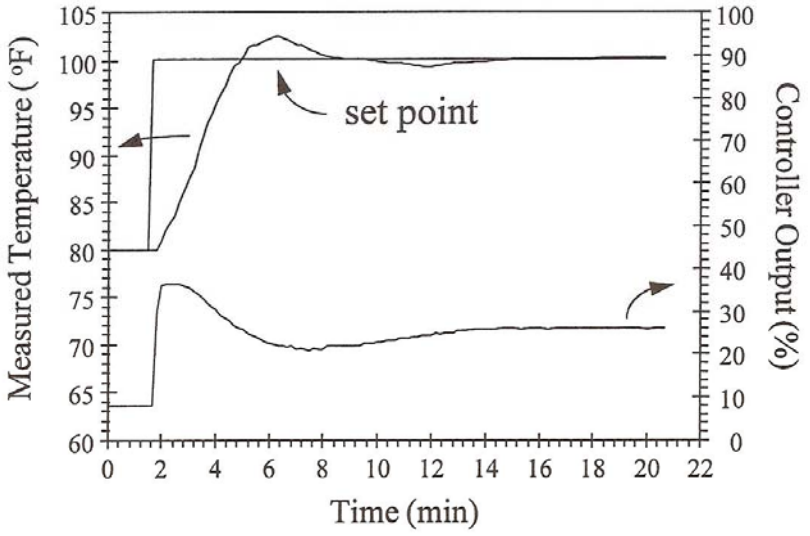


Figure 7. Set point tracking using the Digest tuning parameters

Figure 8 shows the disturbance rejection capability of the controller. The set point was held constant during the experiment at the design value of 90·F. The flow of cold water to the tank (the disturbance variable) was initially set at 2.4 gpm and the process was permitted to steady. The disturbance flow rate was then stepped to 3.6 gpm, thus bracketing the design value of 3.0 gpm. As shown in Figure 8, the controller performs well in rapidly rejecting the disturbance and returning the tank temperature to the set point value.

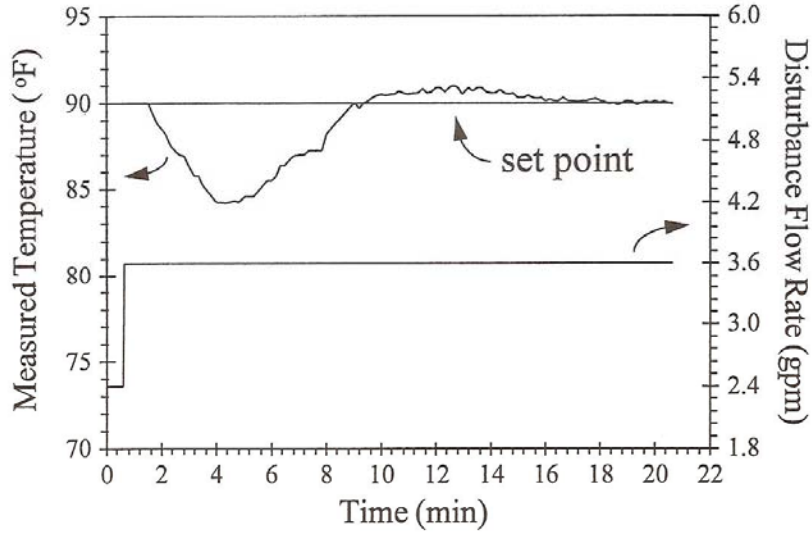


Figure 8. Disturbance rejection using the Digest tuning parameters

More Challenging Data

The simple step test used in the preceding experiment did not really demonstrate Digest's capabilities in modeling process data. Figure 9 shows a somewhat more challenging demonstration, which includes a sequence of manipulated input variable steps followed by two brief sinusoids.

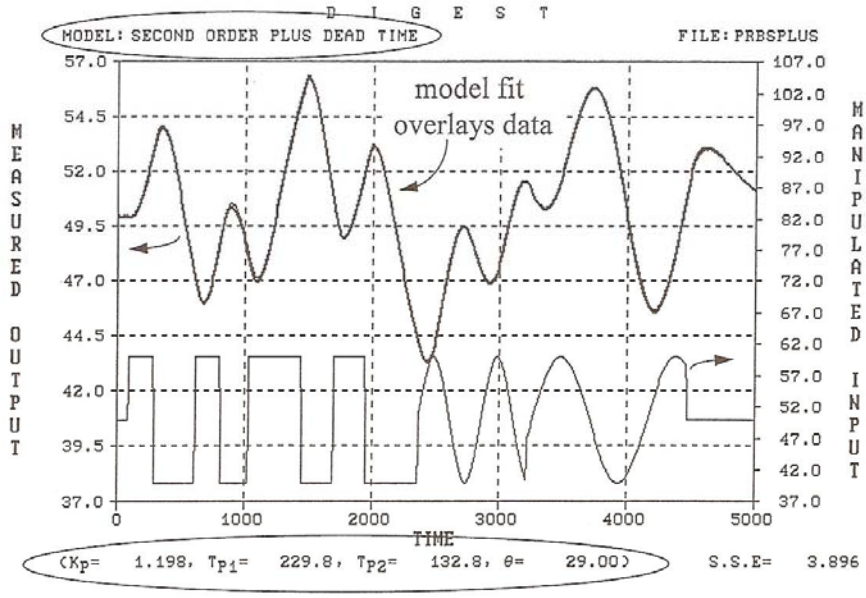


Figure 9. Digest fit of second order plus dead time data

The data was generated from a second order plus dead time (SPODT) simulation using Picles' Design a Process. The process was sampled every 10 seconds. The measured variable data was corrupted with uniform random error which had a standard deviation equal to ± 0.1.

As shown in Figure 9, the Digest fit is so accurate that the model fit overlays the data almost exactly. The Digest model parameters compare to the actual SOPDT values used in Picles as:

Parameter	Actual	Digest Fit
K_p	1.2	1.2
$\tau_{p,1}$	250	230
$\tau_{p,2}$	125	133
θ_p	27	29

Although one of the time constants fit by Digest is slightly smaller than that used in Picles, the other is slightly larger to produce an overall dynamic character which is nearly identical to the actual simulation.

For More Information

Digest is indeed a powerful tool which makes modeling process dynamics and estimating PID controller tuning parameters a quick and easy process. The latest version of Digest now permits unevenly spaced sampled data, an important feature for lab and pilot plant applications.

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

ANNOUNCEMENTS

Changes in Executive Committee

CACHE is pleased to announce these changes in the Executive Committee. The offices of President, Vice-President, and Secretary will be as follows:

President

Lorenz T. Biegler
University of Pennsylvania

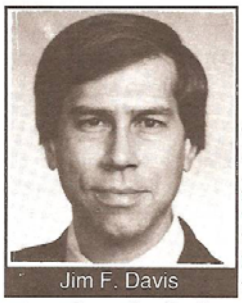

Larry T. Biegler

Lorenz T. (Larry) Biegler is currently the Bayer Professor of Chemical Engineering at Carnegie Mellon University, where he has served on the faculty since receiving his Ph.D. from the University of Wisconsin in 1981. His research interests are in the areas of computer aided process analysis and design and include flowsheet optimization, optimization of systems of differential and algebraic equations, reactor network synthesis and algorithms for constrained, nonlinear process control.

Professor Biegler has been a visiting scholar at Northwestern University, a scientist-in-residence at Argonne National Lab, a Distinguished Faculty Visitor at the University of Alberta and a Gambrinus Fellow at the University of Dortmund. He has authored or co-authored over a hundred technical publications and presented numerous papers at national and international conferences. He received the Curtis McGraw Research Award from ASEE, a Presidential Young Investigator Award from the National Science Foundation, and is listed in Who's Who in Science and Engineering and Who's Who in Engineering. He has held several offices in the American Institute of Chemical Engineers and is also a member of SIAM, ACS and Sigma Xi. Professor Biegler has been a CACHE trustee since 1986 and served as CACHE secretary from 1990 to 1992.

Vice-President

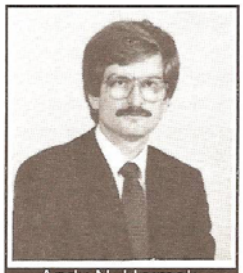
James F. Davis
Ohio State University


Jim F. Davis

Jim Davis is Professor of Chemical Engineering at Ohio State University. He also holds the position of Associate Provost and Director of University Technology Services with responsibility for strategic planning in information technologies and for central computing and technology support operations. He came to Ohio State University with industrial experience at Amoco Chemicals Corporation and Argonne National Laboratory. Since the early 1980s, Jim's research work has been focused in the area of Intelligent Systems in process operations and design. The work has led to the implementation of a number of intelligent decision support systems in a variety of industrial applications. Jim has made numerous presentations and published extensively in the area. In addition he has consulted widely in the areas of knowledge-based systems and neural networks. Jim has been a CACHE trustee for almost 10 years and has served on the executive committee. Jim has also been active in the AIChE for many years including area programming activities, chairing technical sessions and CAST Director from 1990-93.

Secretary

Andrew N. Hrymak
McMaster University


Andy N. Hrymak

Andy is a Professor of Chemical Engineering at McMaster University in Hamilton, Ontario, Canada. He completed his B.Eng. at McMaster and his Ph.D. at Carnegie Mellon University. Courses taught include: process flowsheeting, optimization, computational fluid dynamics and polymer processing. His research interests are in process modeling and optimization, computational fluid dynamics (especially with free and moving boundary value problems) and 3-D models for polymer processing applications. Current research projects include multilayer flows of polymer melts and solutions, twin screw extruder models, real-time optimization and scheduling of batch and continuous processes and the development of brownstock pulp washing fundamental models. Andy has been an Academic Trustee of CACHE Corp. since 1991.

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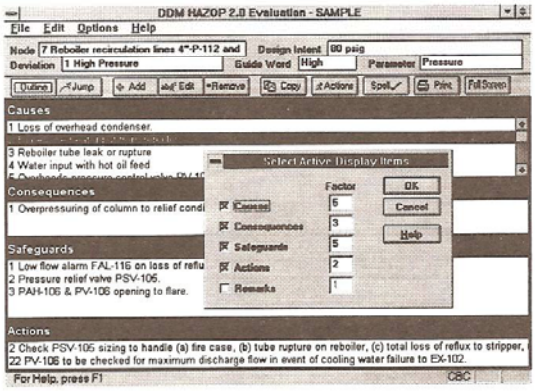

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POLYMATH 4.0 Update

The latest version of POLYMATH is now available from the CACHE office. An order form is attached to this article. All users who have a continuing site license should have received this latest version. Please contact the CACHE office if you have not. There is also a special offer of a POLYMATH trial period for three months for an academic department before a site license needs to be purchased. Details are also at the end of this article.

A number of improved and enhanced features are now provided. Polymath programs now include capabilities for

1. Simultaneous Ordinary Differential Equations
2. Simultaneous Nonlinear Equations
3. Simultaneous Linear Equations
4. Polynomial, Linear and Nonlinear Regressions

with the separate Linear Equation Solver being a new program.

Number of Equations/Lines per Equation

Most experienced users will appreciate that the **number of equations** has been increased to 31 and up to three **lines per equation** are now allowed in the first two of the POLYMATH programs. These capabilities will allow much more complicated problems to be solved.

Logical Variables

An important new capability is the unlimited use of **logical variables** in the differential and nonlinear equations programs. This allows an IF, THEN, ELSE logic to specify changes in any of the program variables. A variety of operators can be used including >, <, >=, <=, == (equals), <> (does not equal), | (or), and & (and). Since nesting is allowed with logical variables, a great deal of flexibility is afforded by this functionality. This is discussed in an article entitled Nonideal Reactor Design Using POLYMATH 4.0 in this newsletter.

Intrinsic Functions (Consistency with Calculator)

A number of intrinsic functions have been added, and there is now consistency between the POLYMATH calculator and all of the POLYMATH programs. Now included are most of the trigonometric functions and their inverses, the hyperbolic functions and their inverses, plus more useful functions. These are discussed in the README.TXT file with the POLYMATH software, in the help sections, and in the manual.

Improved Numerical Algorithms

The Differential Equations Solver now has improved integration algorithms. For nonstiff problems, the Runge-Kutta-Fehlberg (RKF) algorithm, with error estimation and step-size control, is used. There is no lower limit on the step size (other than machine precision). The program will decrease the step size in order to achieve a relative and absolute error or 10^{-10} if possible. If an accuracy becomes less than 10^{-4}, then the user can choose a "semi-implicit midpoint rule" which is an algorithm for stiff problems.

Expanded Statistical Output for Regressions

More statistical information is now provided in the various regressions involving polynomials, multiple linear functions and general nonlinear functions. This includes the matrix of correlation coefficients, the 95% confidence intervals for all parameters, residual plots, and the overall variance. This can be quite useful in deciding which model should be retained and used to correlate data.

Improved Graphical Output and Support for Printers, Plotters and Graphics Files

Most of the graphical results can be edited to change the scales of the x and y axes, to label the x and y axes, and to title the graph. Normal printing is to a variety of some 30 standard printers and six plotters. Advanced printing options provide a variety of standard graphical file types for incorporation into documents.

POLYMATH Trail Offer

The new version 4.0 of POLYMATH has capabilities which greatly enhance the usefulness of the software. Students and faculty find the software particularly easy to learn to use. Details on ordering POLYMATH are given below. There is no risk in evaluating this software. The inexpensive site license allows unlimited copying of the software for educational use by students, faculty and staff. You may request this package from CACHE for testing and evaluation. If you decide to obtain POLYMATH for possible classroom or departmental use, please note the conditions indicated on the order form on the next page.

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POLYMATH Order Form

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

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2. Your department chairman will be informed of the testing.
3. 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.

Please send me a copy of POLYMATH for the IBM/PC. I have read and understood the conditions described above.

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ANNOUNCEMENTS

New CACHE Product

*MultiBatch*DS Educational Version 2.0

by Urmila Diwekar
Carnegie Mellon University

The recent increase in the production of high value-added, low-volume specialty chemicals and biochemicals has generated a renewed interest in batch processing technologies. Batch distillation is an important unit operation in the batch processing industry and is widely used. The flexibility of batch distillation, combined with the inherent unsteady nature of the process, poses challenging design and operation problems. In view of the practical importance of batch processing and in response to industrial demands for chemical engineers with a strong background in batch processing, more and more educational institutions are redesigning their curricula to include courses devoted to the subject.

A dedicated course on batch distillation will (a) introduce the various configurations of conventional and emerging batch distillation columns, (b) examine the challenges involved in a rigorous modeling of batch distillation column dynamics, (c) describe the various operating modes in detail, (d) provide hierarchy of models of varying complexity and rigor, (e) present approaches to optimal design of batch distillation and highlight the differences vis-à-vis continuous distillation columns, (f) described optimal control algorithms and its application to batch distillation, (g) discuss analysis and synthesis of columns with complex thermodynamics, and complex, unconventional column configurations, and (e) illustrate real-world applications.

It is difficult to teach batch distillation without using computers due to the two reasons stated above: (1) the process is time varying and one has to resort to complex numerical integration techniques and different models for obtaining the transients, and (2) this ever-changing process also provides flexibility in operating and configuring a column in numerous ways. *MultiBatchDS* is a general purpose batch distillation package that can be used for understanding batch distillation process principles. The principles of the batch distillation process are more easily understood through simple thermodynamic models. Therefore, the educational version of the package comes with a constant relative volatility model, as well as a databank of 103 commonly used chemical components. For components in the databank one can choose the ideal fugacity models or the models based on the UNIFAC method for nonideal fugacity calculations. The databank and thermodynamic models were provided courtesy of Dr. Gani in the Department of Chemical Engineering at the Technical University of Denmark.

MultiBatchDS will be available for purchase from the CACHE office approximately November 1, 1996.

MultiBatchDS Educational Version 2.0

MultiBatchDS Educational Version 2.0 consists of two diskettes for the PC. They contain a copy of the program along with help files including tutorials and example problems. There is also a manual available at an extra cost of $10.00. There will be a yearly license fee of $90.00 to use the program. See Standard Order form.

ANNOUNCEMENTS

*MultiBatch*DS Educational Version 2.0

MultiBatchDS: Professional Batch Distillation Systems for multiple column configurations, multiple operating modes, multiple fractions, and multiple products—with multiple levels of models

Complete 32-bit integrated visual environment on your PC or workstation running under Windows 95 or NT for simulation, optimal design, and control of batch distillation systems. You have the power of on-line monitoring and control of program execution. Change configuration, operating mode, or any parameter and see *MultiBatchDS* recalculate the output—It's that easy.

MultiBatchDS can be used for understanding batch distillation principles.

Technical Highlights

Conceptual Design

- Simple-yet-effective models for preliminary design, synthesis, optimization, and rapid analysis of column behavior.
- Design feasibility analysis.

Column optimization and optimal control

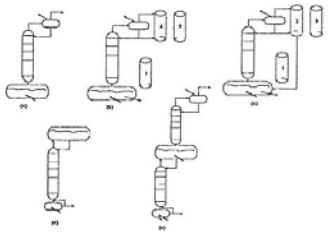
- Solution of maximum distillate, minimum time, or maximum profit problems.

Numerical Methods

- Robust algorithms for non-stiff and stiff systems.
- Model switching for highly stiff systems
- Collocation models for partial differential equation systems including packed columns
- Rigorous error handling.
- 32-bit implementation of the complete calculation engine and user interface for better performance and large scale problems.

Modeling

- Capabilities for analyzing and optimizing complex and unconventional column configurations, including emerging designs such as columns with a middle vessel and stripper.



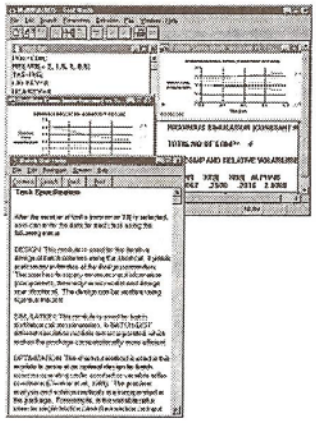
Different column configurations including emerging designs

- Rigorous models for detailed column design based on solution of fundamental equations governing transient heat and mass transfer column operation.
- Simulation of startup conditions.
- Dynamic simulation models with varying degrees of complexity and rigor.
- Various modes of operation like constant reflux, constant reboil ratio, variable reflux, variable reboil ratio, optimal reflux, and optimal reboil ratio. Possibility of analyzing side feeds and side products.
- Databank and thermodynamic models for predicting properties and vapor-liquid equilibria of ideal and nonideal mixtures.

configure • simulate • design • optimize • control multicomponent batch distillation systems

Visual Highlights

- A user-friendly graphical input interface based on Windows 95 and Windows NT. Also supports keywo input structure where commands can be written in simple English.
- Flexible and easy-to-use menus and sub-menus.
- Powerful, interactive plotting with multiple options f abscissa and ordinate for each fraction.
- Graphical as well as textual output results.
- Extensive error checking and reporting.
- On-line help screens.
- On-line monitoring and control of the program execution.



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1996 ASEE Award Winner

The CACHE Corporation and the Chemical Engineering Division of ASEE

presented the 1996

Excellence in Computing in Chemical Engineering Award

to

Kenneth R. Jolls

for outstanding contributions

CACHE CD-ROM's

CACHE CD-ROM - Volume 2 is now available from the CACHE office.

There are a few remaining copies of the CACHE 25th Anniversay CD-ROM - Volume 1 still available from the CACHE office

See Standard Order Form

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