ChE *classroom*

CREATE *VIRTUAL* UNIT OPERATIONS WITH YOUR DATA ACQUISITION SOFTWARE

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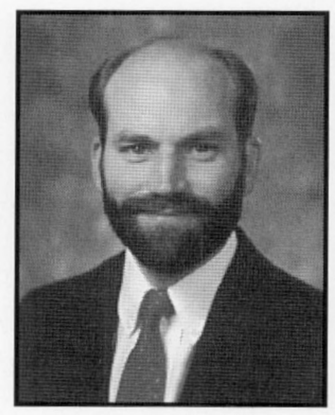

The latest generation of computer data acquisition software and hardware for personal computers allows for simple and inexpensive, yet powerful, automation of laboratory experiments and process control.[1-4] But modern data acquisition software can also serve as a convenient tool for quickly developing computer simulations of chemical engineering unit operations for use in classroom demonstrations.

Recently, several different types of computer data acquisition software with a graphical user interface (GUI) have become commercially available, including National Instrument's LabVIEW, VIEWDAC from Keithly Metrabyte, Labtech Notebook and Control, and Kmax from Sparrow, among others. These computer applications are designed to replace physical instrumentation with virtual instruments (VI).

A VI permits the user to access the functions of computer data acquisition hardware (*e.g.,* plug-in cards) with programmable software that graphically portrays the controls and output as knobs, buttons, switches, thermometers, and strip charts on the computer's video display. The advantage of creating simulations using data acquisition software with a GUI over traditional programming languages like FORTRAN or BASIC, or even mathematical analysis applications such as Mathematica or Mathcad, is the availability of pre-drawn controls and output devices,[5,6] similar to those found in visualization and simulation software packages like SIMULINK and VisSim.

A typical example of a GUI is shown in Figure 1, where the general feel and appearance of physical instrumentation is created with computer graphics. The controls, however, are manipulated with the "click and drag" of a computer mouse. All of these features make data acquisition software ideal for creating VIs of unit operations. The powerful programming, analysis tools, graphical interface, and presentation graphics can be combined to simulate, in real time, the operation and dynamic behavior of several different unit operations involving fluid dynamics, heat transfer, separations, or reactor design.

We purchased LabVIEW for use in a research setting, but found it particularly well suited for creating VIs of unit operations for classroom demonstrations as well. LabVIEW is essentially a high-level programming language, available for Macintosh, Windows, and UNIX platforms. LabVIEW replaces text-based programming with icons or object-oriented programming. In addition to objects for data acquisition and control, LabVIEW comes with an extensive library of numerical and statistical analysis tools. With the latest version of LabVIEW, software developers can create stand-alone, executable only applications that can be distributed freely.

Goodney[7] first reported success using LabVIEW in the analytical chemistry classroom for simulating the collection and analysis of absorption peaks from chromatographic separations. More recently, using similar data-acquisition soft-

ware, LabWindows (also from National Instruments), Dempster[8] developed a series of simulated laboratory experiments for physiology and pharmacology undergraduate students, such as drug delivery in a cat. While our needs are not so animated, with relatively little programming effort, VIs of unit operations such as heat exchangers, stirred reactors, and absorption towers were created with LabVIEW for use as classroom demonstrations. One VI of a stirred tank reactor (STR) is presented here in order to illustrate the features of simulation with data-acquisition software. This simulation is designed to demonstrate the effects of several process parameters on temperature and reaction conversion in a stirred tank reactor.

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VIRTUAL STIRRED TANK REACTOR

A dynamic simulation of a stirred tank reactor is developed to demonstrate both batch versus continuous operation (or chemical equilibrium versus steady state), non-ideal mixing, and residence time effects on temperature and conversion in a reactor. The details of the model derivation may be found in any standard textbook on reactor design.[9]

For simplicity, the model is formulated for the simple case of an elementary, first-order, reversible, constant density, exothermic reaction:

$$A \underset{k_{-1}}{\overset{k_1}{\Leftrightarrow}} B \qquad (1)$$

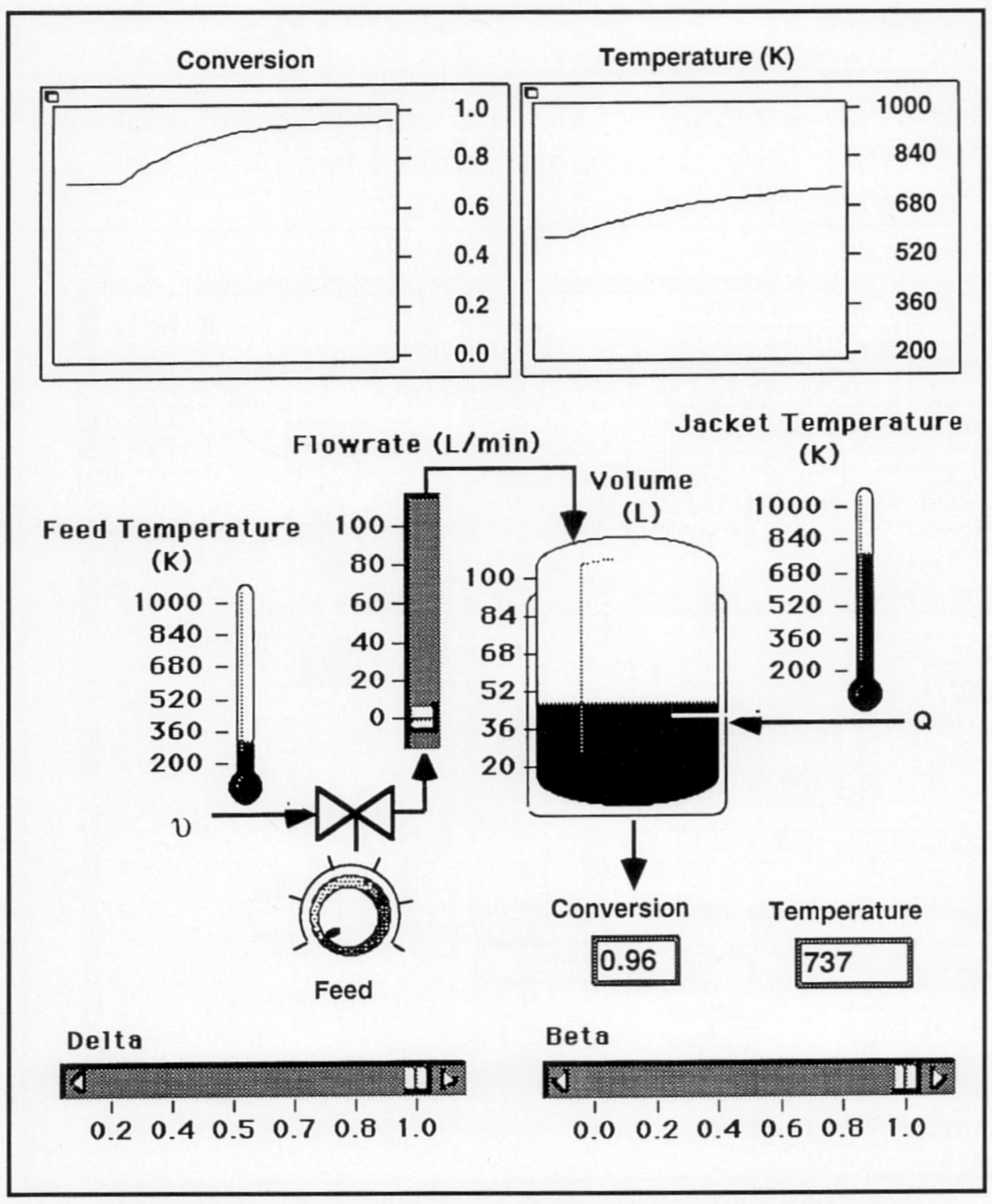

Figure 1. *Simulation graphical user interface.*

The elementary rate law for this reaction is

$$-r_A = k_1\left(C_A - \frac{C_B}{K}\right) \qquad (2)$$

The first-order rate constant taken to be Arrhenius temperature dependent is

$$k_1 = k_{10}\exp\left(\frac{E}{RT}\right) \qquad (3)$$

where k_1 is the forward rate constant and K is the reaction equilibrium constant, defined as

$$K = \frac{k_1}{k_{-1}} \qquad (4)$$

An Arrhenius temperature dependence is also assumed for the equilibrium constant

$$K = K_0\exp\left(\frac{E_e}{RT}\right) \qquad (5)$$

Conservation Equations • Several assumptions are introduced into the model to keep the derivation simple. The feed is pure A and the density of the reactant and product are constant and uniform. Under these conditions, the unsteady-state material balance for species A is

$$V\frac{dC_A}{dt} = \upsilon\left(C_{Ao} - C_A\right) + Vr_A \qquad (6)$$

where

V = reactor volume
υ = volumetric feed rate
C_A, C_{Ao} = reactor and feed concentrations, respectively
r_A = reaction rate of species A

The concentration of each species is defined in terms of the conversion of species A:

$$C_A = C_{Ao}(1 - X) \qquad (7)$$

$$C_B = C_{Ao}X \qquad (8)$$

The species conservation Eq. (6) reduces to the following first-order ordinary differential equation in conversion:

$$\frac{dX}{dt} = k_1 - X\left[k_1\left(1 + \frac{1}{K}\right) + \frac{\upsilon}{V}\right] \qquad (9)$$

Deviations from perfect mixing are illustrated with this model by modifying Eq. (9) to account for non-ideal behavior. One

simple two-parameter model of a non-ideal mixing is a stirred tank reactor with a bypass stream and dead volume, as illustrated in Figure 2. In this case, the modifications to the conservation equation for dead volume and bypass give

$$\upsilon_b = (1-\beta)\upsilon \tag{10}$$

$$V_d = (1-\delta)V \tag{11}$$

$$\frac{dX_1}{dt} = k_1 - K_1\left[k_1\left(1+\frac{1}{K}\right)+\frac{\beta\upsilon}{\delta V}\right] \tag{12}$$

$$X_2 = \beta X_1 \tag{13}$$

where X_1 is the conversion in the non-ideal reactor and X_2 is the total conversion, including the effects of bypass. The reactor model is also set up with a uniform temperature jacket for temperature control. The thermal energy conservation equation is

$$\frac{dT}{dt} = \frac{US(T_\infty - T)}{C_{Ao}c_p\delta V} + \frac{\beta\upsilon}{\delta V}\left[(T_0 - T) - \frac{XH_r}{c_p}\right] \tag{14}$$

where

US = product of the overall heat transfer coefficient and area available for heat transfer

T_∞, T = jacket and reactor temperatures, respectively

H_r = heat of reaction

c_p = heat capacity of the fluid

Simulator • The STR VI simulation's controls and results are displayed graphically by LabVIEW on a Macintosh computer as shown in Figure 1. The model equations are solved numerically in a LabVIEW program shown in Figure 3. In order to keep the programming compact, a simple first-order Euler's method is used to solve the system of first-order ordinary differential equations for this example. The discrete form of Eqs. (12) and (14) are contained in a formula node that is placed inside an overall while-loop structure. A feature of this simulation is the ability to run in real time, accomplished by controlling the time elapsed between while-loop iterations with a wait period (represented by the small clock in the lower right-hand corner) equal to the Euler time step. The time elapsed is controlled by the internal clock on board the computer. The smaller formula node is used to calculate values for the Arrhenius temperature dependent reaction rate and equilibrium constants.

LabVIEW comes with several pre-drawn control and output options. Virtual thermometers are used for temperature indicators and controllers. In this particular VI, the temperatures of the feed stream and jacket are controlled directly from the screen by dragging the virtual mercury up and down the thermometers, using the computer's mouse. A virtual filled tank is used to represent the reactor and its volume is controlled in a similar fashion, using the computer's mouse to drag the volume level in the icon up or down. The feed flow rate is controlled with a virtual knob. A rotameter indicates the value of the flow rate. Slide bars are used for changing the bypass and dead volume fractions for incorporating non-ideal mixing into the simulation. Strip charts record the dynamic results for conversion and temperature from the reactor simulation. Controls and strip charts are "wired" to their respective variables used in the formula nodes in Figure 3. Although not shown in Figure 1, the values of all the parameters, such as activation energy and heat of reaction, may be changed by typing the appropriate numbers in digital

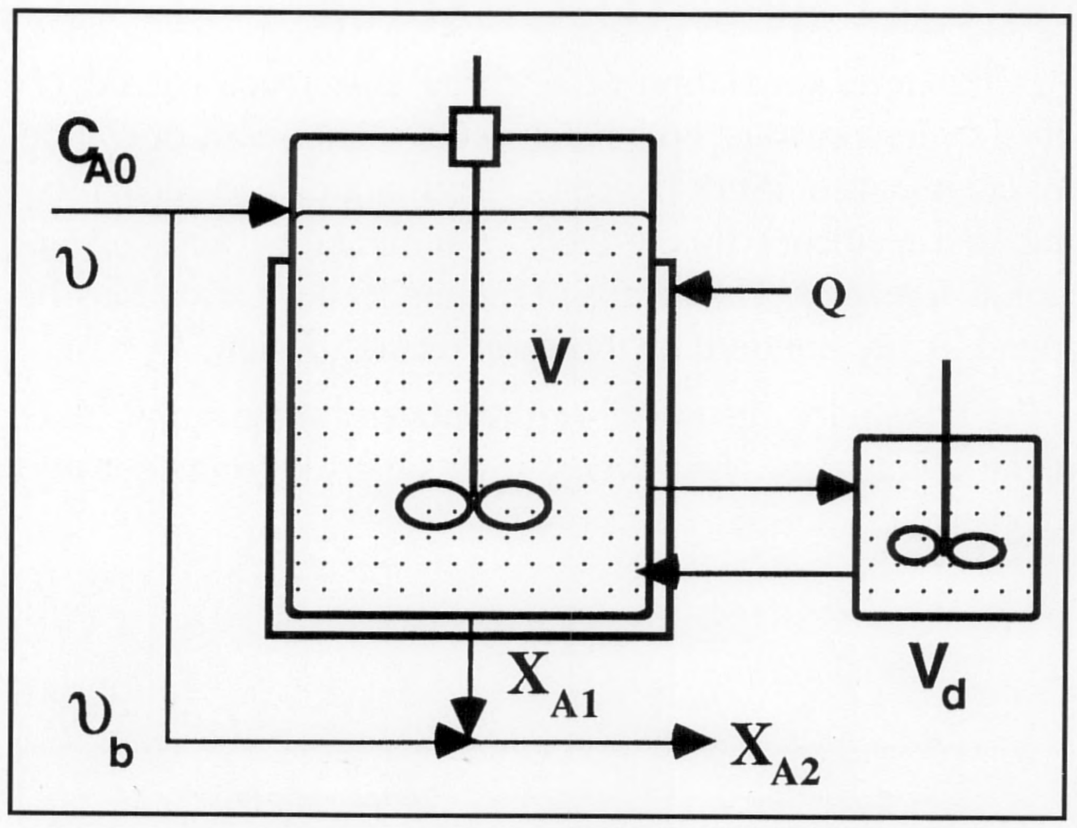

Figure 2. *Schematic of jacketed stirred tank reactor with by-pass stream and dead volume.*

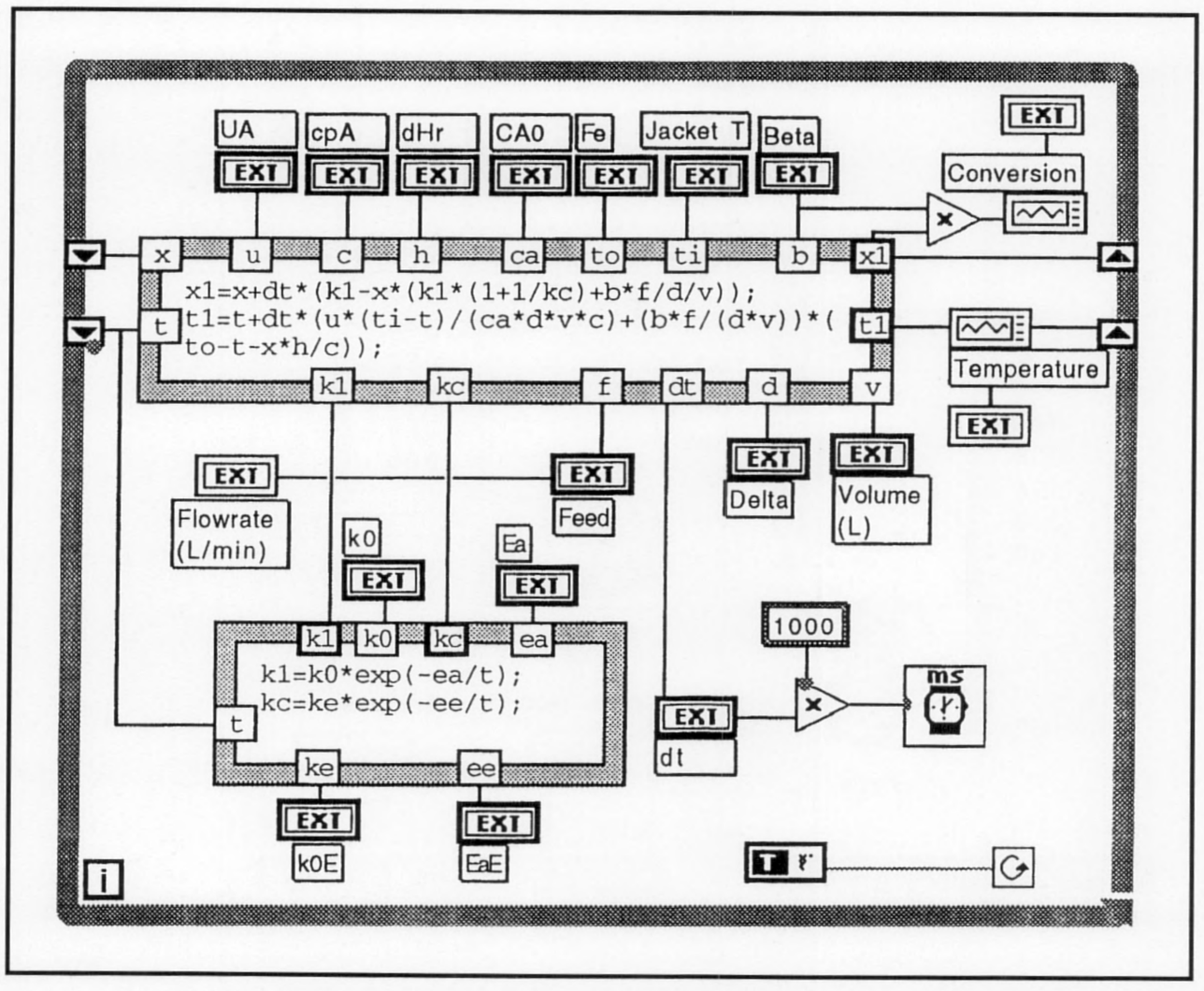

Figure 3. *Icon-based program for STR simulation.*

control boxes. The values of the parameters chosen for this simulation are listed in Table 1.

Computer simulations of unit operations allow us to investigate the effect of changing parameters that would otherwise be impossible. For example, the effect of activation energy on temperature dependence is demonstrated on-line by varying the activation energy and temperature over a range of values and plotting the results in the strip charts created by the software.

SAMPLE SIMULATIONS

Several simulations are possible with this single STR VI. They range from the simple investigation of the transient temperature of a batch reactor to the effects of mixing on the conversion of a first-order reaction.

Table 1
Parameter values for STR simulation

Reaction	*Parameters*
k_1	50 min^{-1}
K	150
C_{A0}	0.1 $mol \cdot L^{-1}$
E/R	1234 K
E_e/R	1357 K
c_p	100 $J \cdot mol^{-1}K^{-1}$
H_r	-10 $J \cdot mol^{-1}$
US	1500 $J \cdot K^{-1}$
Δt	0.02 s

Students often have difficulty distinguishing between the concepts of steady state and equilibrium operation. By turning off the feed flow rate in the STR simulation, the continuous reactor becomes a batch reactor. The strip charts in Figure 1 show the results of the dynamic effects on conversion and temperature when the feed is set to zero. At early times, the reactor is operating under steady-state conditions, represented by the flat concentration and temperature profiles. When the feed is stopped, the steady-state conditions become the initial conditions for batch operation. At this point in time, conversion and temperature in the reactor begin to increase asymptotically toward their equilibrium state, illustrating the transient nature of batch operation. Unfortunately, the figures shown here are only still snapshots of the output, diminishing the visual impact of the dynamic computer video output that students see in class.

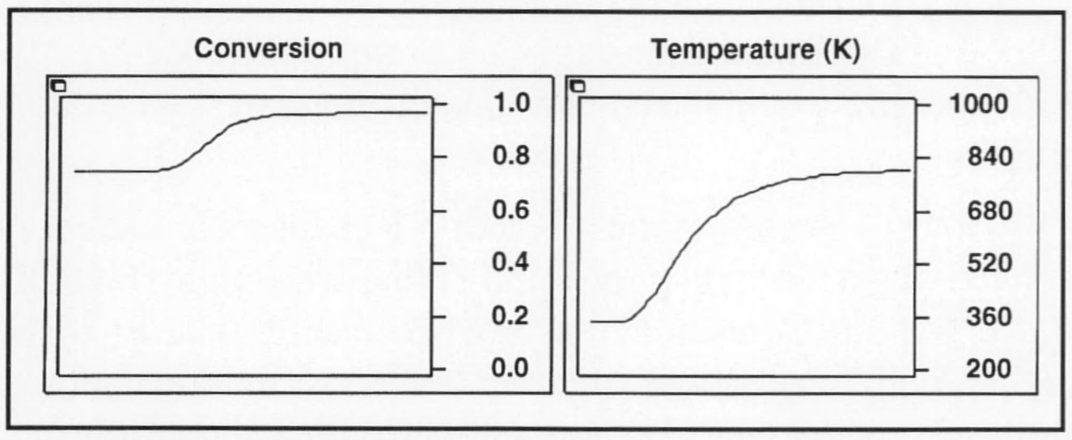

Figure 4. *Temperature effects on equilibrium in a batch reactor.*

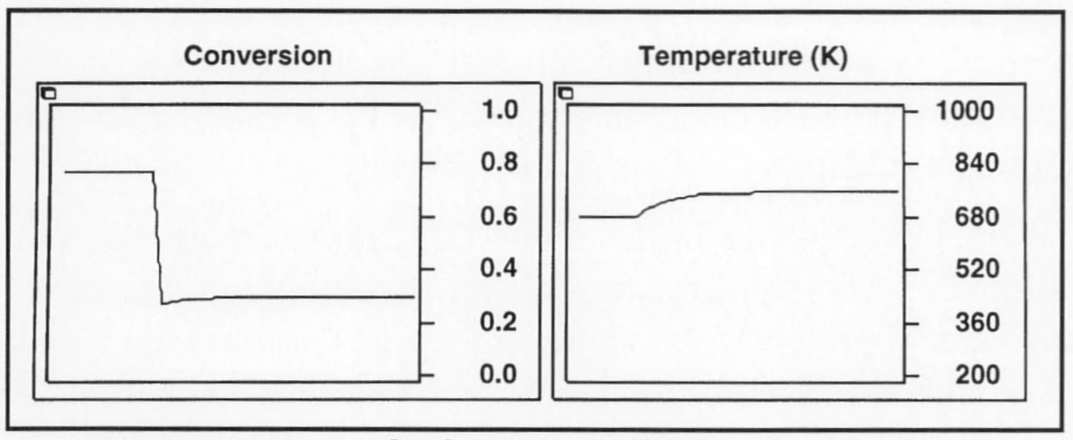

Figure 5. *Non-ideal mixing effects on conversion and temperature.*

The effect of temperature on equilibrium is demonstrated by adjusting the temperature of the heat exchanger fluid in the jacket. Figure 4 shows the strip charts for conversion and reactor temperature under batch operation when the jacket temperature is increased from 350 to 800 K. The conversion gradually increased from 75% to 96%.

The influence of residence time on conversion and temperature is illustrated by changing either the feed flow rate or the reactor volume. A lower flow rate increases conversion while decreasing production rate. Depending on the temperature of the feed stream, the temperature in the reactor decreases or increases as the residence time is changed.

Students can explore different scenarios in class by asking "What if ... ?" questions about the effects of each controllable parameter on conversion or temperature in the reactor. For example, students ask how the production rate can be increased without loss of conversion. One possibility is to increase the reactor volume while increasing the feed rate, but this may have an effect on the degree of mixing, which leads into a discussion of mixing models. The ideal mixing model is altered to account for stagnant regions and channeling in the reactors. Step changes from 1.0 to 0.5 in β and δ result in the transient conversion and temperature plots in Figure 5.

Another typical question concerns the activation energy effects on the temperature dependence of the reaction. This is typically demonstrated in the physical chemistry or unit operations laboratories only by choosing different reacting compounds for study. In this dynamic simulation, the activation energy as well as the temperature can be changed "on-line" while the program is running. The simple model developed here may be modified to include higher order reactions or other non-ideal reactor models as desired.

DISCUSSION

Although originally intended for automating data collection from a laboratory experiment or process control, modern data acquisition software with a GUI is also a useful and convenient tool for developing computer demonstrations of unit operations. Many chemical engineering departments may have plans for acquiring data acquisition software for automating the unit operations laboratory that can also serve

as a programming aid for computer simulations (giving you twice the bang for your educational or research buck!). Mathematical models can be programmed with graphical displays for control and output to illustrate the salient features of many unit operations, such as the stirred tank reactor demonstrated here.

Of particular benefit to students is the ability to demonstrate unsteady-state behavior in real time. I have found that the difference between equilibrium and steady state is often a difficult concept for students to grasp. The student response to this simulation is generally favorable. The computer demonstrations are portable, inexpensive when coupled with laboratory use, and require minimal effort to customize for particular needs. National Instruments offers special academic pricing on LabVIEW as well as a low-cost student edition. Interested departments should contact National Instruments directly for more information.[10]

NOTATION

C_A = concentration of species A
C_{A0} = feed concentration
C_B = concentration of species B
c_p = heat capacity
H_r = heat of reaction per mole of species A
E = activation energy for reaction rate constant
E_e = activation energy for equilibrium constant
K = reaction equilibrium constant
k_1, k_{-1} = first-order forward and reverse reaction rate constants
k_{10} = pre-exponential factor for k_1
R = ideal gas constant
r_A = reaction production rate of species A
S = heat transfer area
t = time
T = reactor temperature
T_∞ = heat exchanger fluid temperature
U = overall heat transfer coefficient
V = total reactor volume
V_d = dead volume
X = conversion of species A from an ideal reactor
δ = fraction of volume converted to dead volume
β = fraction of feed converted to by-pass stream
Δt = Euler step size in numerical solution
υ = volumetric feed flow rate
υ_b = by-pass volumetric flow rate

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REVIEW: *Studying Engineering*

Continued from page 229.

part-time work agrees with my experience. The book encourages students to seek help and to work together in collaborative groups with an optimum size of two. His suggestions on how to get help from professors is good, but will drive professors at research universities crazy if a large number of students start to follow his suggestions. The study skills will be useful if the students practice them. The problems at the end of the chapter will be helpful here, particularly if assigned as homework.

Chapter 4, "Developing Yourself Personally," presents one major message—think positively. A section on the three steps to overcoming barriers is outstanding. These three steps (Knowledge, know what to do; Commit, want to do it; and Implement, do it) will be useful to professors as well as to students. Unfortunately, five pages on Maslow and self-esteem, two pages on the Myers (which he misspells)-Briggs Type Indicator, and four pages on brain dominance are all too short and would have to be supplemented by the instructor.

Chapter 4 seems to be a catch-all chapter. It includes sixteen pages on communication skills, with many helpful hints. But since freshman engineers typically take English and speech, why devote so much space to communication? A short section to provide motivation would have been sufficient. A section on understanding and respecting differences reflects the author's experience as director of a minority engineering program. Because of the importance of this topic, I wish it were longer and that it included role plays or scenarios. The final section on motivating yourself could be moved to Chapter 1 where it fits naturally.

Chapter 5, "Broadening Your Education," suggests that students participate in campus life, participate in engineering student projects, obtain preprofessional employment, and give something back to the school. These are all obviously useful suggestions. The sections on campus life and student projects try to be specific in areas where different schools