ChE curriculum

CHEMICAL ENGINEERING AND INSTRUCTIONAL COMPUTING

Are They In Step?

PART 2

***EDITORIAL NOTE:** Part 1 of this article appeared in the summer 1988 issue of CHEMICAL ENGINEERING EDUCATION and ended with the questions*

- *Can microcomputers stimulate the use of open-ended, design-oriented problems?*
- *Can high-resolution displays permit students to better learn the principles through visualization of streamlines in fluid flows, visualization of PVT, etc?*
- *Can computers enable students to analyze and possibly design less conventional processes involving, for example, crystallization of chips, deposition of thin films, natural convection in solar cells, etc?*

These questions are addressed in this second part of Dr. Seider's paper.

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The stimulus for open-ended problem-solving in the core courses of the undergraduate curriculum arises from the need to expose students to the methods of formulating and solving problems with many alternate solutions. In many curricula, this exercise is reserved primarily for the capstone design course. Yet with highly-interactive computers which require the student to do minimal or no programming, it should be possible to add more open-ended problems to the core courses while more adequately satisfying the controversial requirement of one-half year of course work in design for the accreditation of undergraduate curricula [1].

This has been the basis for the CACHE Corporation project to develop *CACHE IBM PC Lessons for Courses Other Than Design and Control* [2]. In the first phase, six authors prepared their lessons with the restriction of the use of the BASICA language on an IBM PC with a color graphics monitor. No other restrictions were set and, consequently, several different formats evolved, some using extensive color graphics with animation to present new concepts, some presenting a derivation of the principal equations (with interspersed questions to be answered by the student), and most permitting parametric studies

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TABLE 1
CACHE IBM PC Lessons for Courses Other than Design and Control

Lesson (Program)	Authors	Courses in
Slurry Flow in Channels	Freeman, Provine, Dow, Denn Berkeley	*Fluid Mechanics*
Supercritical Fluid Extraction	Kellow, Cygnarowicz, Seider Penn	*Separations and Thermodynamics*
Gas Absorption with Chemical Reaction	Nordstrom, Seinfeld Cal. Tech.	*Separations*
Design of Flash Vessels and Distillation Towers	Finlayson, Kaler, Heideger Washington	*Separations and Thermodynamics*
Heterogeneous Reaction Kinetics	Bauer, Fogler Michigan	*Reactor Analysis*
CSTR Dynamics and Stability	Vajdi, Allen UCLA	*Reactor Analysis*

with graphical output. The six lessons (see Table 1) have recently been distributed on diskettes by the CACHE Corporation.

The lesson for the "Design of a Slurry Pipeline," developed for the fluid mechanics course, presents the student with a mass rate of solids to be pumped a given distance. Using the Frankel-Acrivos equation for the viscosity as a function of composition, he or she must choose the slurry concentration and pipeline diameter to minimize the net present value of the cost over the life of the pipeline. First, the student derives the equations to minimize the power consumption. Then the microcomputer program is used to vary the design parameters interactively and to prepare a family of curves, as illustrated in Figure 1, in which the power is plotted as a function of the solids fraction.

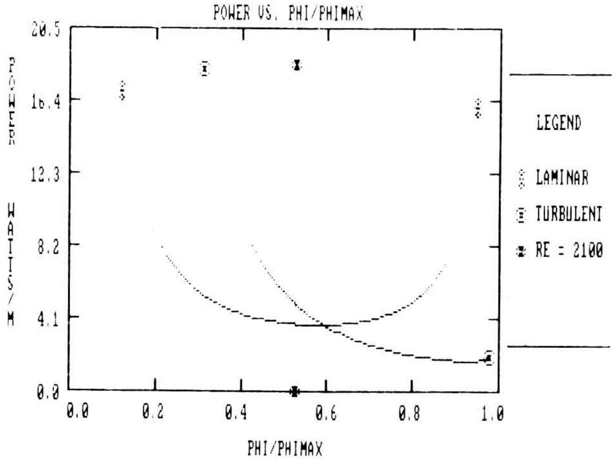
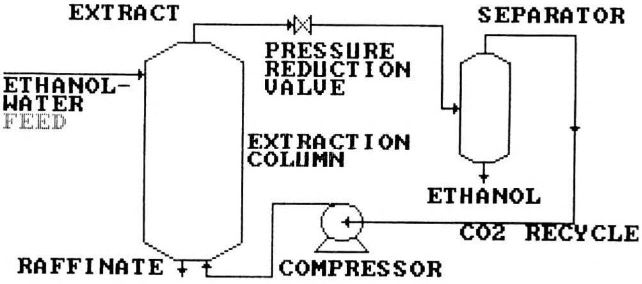
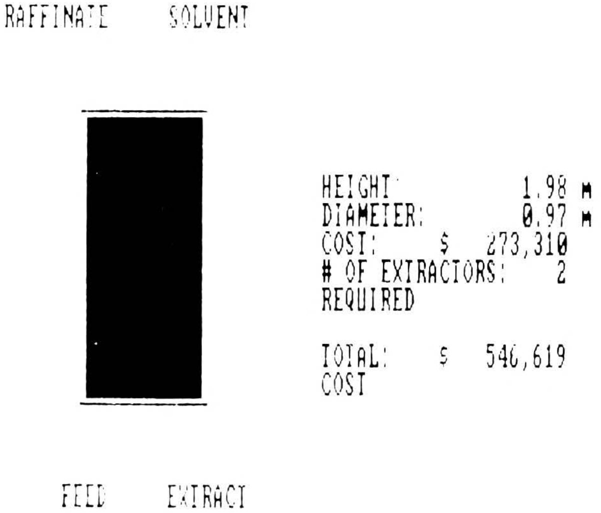


FIGURE 1. Power consumption in slurry flow. From IBM PC lesson for the design of a slurry pipeline [2].

The lesson on supercritical extraction provides approximately fifty frames, some with animation, to introduce the principles of SCE before teaching, by example, the design procedure [3]. The program, which is currently limited to the dehydration of ethanol with carbon dioxide, allows the student to find the optimal design for the flowsheet in Figure 2a. The student guides the program through the procedures that compute the size and cost of the extractor, flash vessel, and compressor. With highly interactive graphics, the student enters the design variables (solvent/feed ratio, flash temperature and pressure, *etc.*) and observes the results in annotated, graphical displays of the process units as well as cost charts. For example, see Figure 2b. The important objectives in the preparation of this lesson included: (1) the provision of an open-ended problem for the separations course that applies the principles to a potentially attractive process, especially when non-toxic solvents are used in food processing, and (2) the use of graphics



(a) Flow sheet for dehydration of ethanol with CO_2



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HEIGHT:          1.98 M
DIAMETER:        0.97 M
COST:      $  273,310
# OF EXTRACTORS:   2
REQUIRED

TOTAL:     $  546,619
COST
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(b) Extractor design

FIGURE 2. Supercritical fluid extraction lesson [2].

and animation to present new material, enabling the student to monitor complex calculations in a way that conventional text books are unable to accomplish.

A third lesson focusses on the dynamics and stability of a CSTR with a first-order, exothermic reaction and heat transfer to a cold reservoir. It begins with an introduction of the concepts of CSTR multiplicity, stability, and dynamics. The basic equations are derived with interspersed questions. Then the student varies the key parameters and the program locates the steady-state nodes and foci and limit cycles, when they exist, and plots the dynamic performance. One such plot is shown in Figure 3. While this lesson doesn't involve a cost function, it exposes the student to the vagaries of exothermic reactor design through instruction in the principles of stability analysis and parameterization. Such an analysis, which has often been regarded as beyond the scope of undergraduate reactor courses, can now be presented to the student without consuming valuable lecture time.

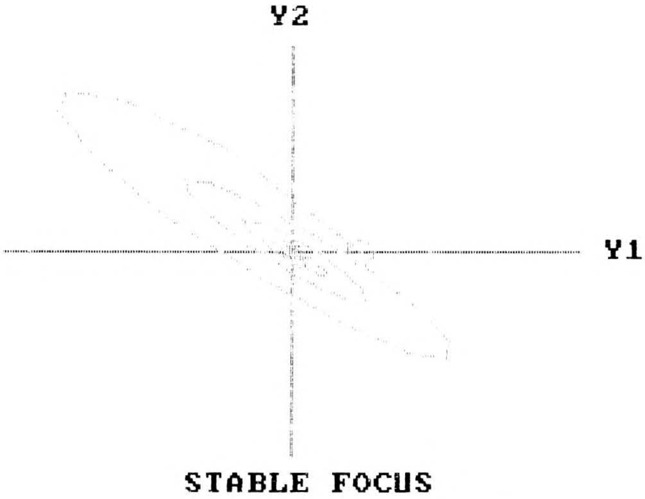


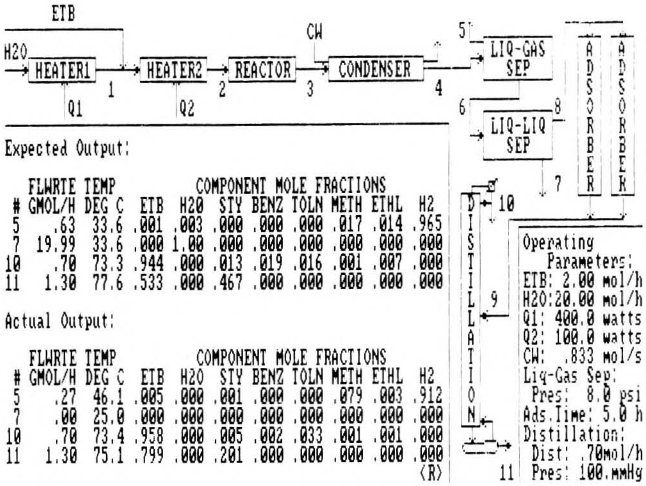
FIGURE 3. Phase-plane of a CSTR with a first-order, exothermic reaction and heat transfer (Y1 = conversion, Y2 = product T). From IBM PC lesson on CSTR dynamics and stability [2].

It should be noted that the six CACHE IBM PC lessons were developed, for the most part, on an experimental basis, often by student programmers, with little or no remuneration. Hence, it is reasonable to expect that they will not entirely fulfill their objectives. Perhaps they will be most useful in presenting examples of what can be accomplished with highly-interactive microcomputers, as well as in having provided the authors experience in the preparation of CAI software.

It is also noteworthy that BASICA was the programming language and that no utility routines were provided for creating the menus, text screens, graphical screens with animation, quizzes, *etc.* Hence, it was necessary to create these facilities in the BASICA language. This resulted in as many as 1200 hours being required to prepare interesting and challenging sequences which use color and animation, avoid repetition, give the students much control, *etc.*

In parallel, several "authoring systems" were being developed in which these and other utility routines are provided for the authors of CAI lessons. MICROCACHE [4], developed at the University of Michigan, keeps records of student usage and performance much more completely than the commercial systems we examined. The latter include the UNISON system [5] by Courseware Applications, Inc., which the CACHE Curriculum Task Force has judged to be the most cost-effective for its next set of CAI lessons (currently in preparation). Others are the PLATO PCD3 (CDC), TENCORE (Computer Teaching Corp.), and CSR Trainer 4000 (Computer Systems Research) Authoring Systems.

In summary, it seems reasonable to answer the question *"Can microcomputers stimulate the use of open-ended, design-oriented problems?"* in the affirmative. Microcomputers *are* beginning to stimulate the use of open-ended problems in the core courses. The cost of software development, principally in student and faculty time, continues to be high. But, the new authoring systems have the potential to sharply reduce the cost and associated effort.



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Expected Output:

  FLWRTE TEMP             COMPONENT MOLE FRACTIONS
 # GMOL/H DEG C  ETB  H20  STY BENZ TOLN METH ETHL  H2
 5    .63  33.6 .001 .003 .000 .000 .000 .017 .014 .965
 7  19.99  33.6 .000 1.00 .000 .000 .000 .000 .000 .000
10    .70  73.3 .944 .000 .013 .019 .016 .001 .007 .000
11   1.30  77.6 .533 .000 .467 .000 .000 .000 .000 .000

Actual Output:

  FLWRTE TEMP             COMPONENT MOLE FRACTIONS
 # GMOL/H DEG C  ETB  H20  STY BENZ TOLN METH ETHL  H2
 5    .27  46.1 .005 .000 .001 .000 .000 .079 .003 .912
 7    .00  25.0 .000 .000 .000 .000 .000 .000 .000 .000
10    .70  73.4 .958 .000 .005 .002 .033 .001 .001 .000
11   1.30  75.1 .799 .000 .201 .000 .000 .000 .000 .000
                                                    <R>
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Operating
   Parameters:
ETB: 2.00 mol/h
H20:20.00 mol/h
Q1: 400.0 watts
Q2: 100.0 watts
CW:  .833 mol/s
Liq-Gas Sep:
 Pres:  8.0 psi
Ads.Time: 5.0 h
Distillation:
 Dist: .70mol/h
 Pres: 100.mmHg
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FIGURE 4. Styrene microplant before and after random generation of a fault [6].

. . . job opportunities are shifting toward the manufacture of silicon chips, the processing of pharmaceuticals and foods, the manufacture of solar collectors, *etc.*, and chemical engineers are being challenged to develop new sensing devices that provide better data and more detailed models to clarify their processing mechanisms.

FAULT DETECTION

While on the subject of interactive microcomputers in undergraduate coursework and before turning to the next question, a program by Heil and Fogler [6] that enables students to detect faults in a styrene microplant is an extraordinary example of a chemical engineering mystery (comparable to the well-known SNOOPER TROOPS detective game). This program is intended to teach the basics of structured problem-solving using the Kepner and Tregoe Method [7]. Through many frames, the student is presented with information concerning the normal operation of the microplant and its performance after a failure has been randomly generated. See, for example, Figure 4. Given $2500, the student must locate the fault, while spending as little money as possible. Detailed information about each process unit is available at no cost. However, when necessary, the student can make experimental measurements at costs between $50-$200. At some point, the student selects from approximately 75 possible faults, thereby initiating repair work at costs between $200-$800. Mistaken diagnoses are charged the full cost of repairs and, hence, it is important to carefully isolate the fault before reporting it.

It is noteworthy that several researchers are seeking methods to automate the fault detection strategies through the use of logic-based, expert systems [8].

HIGH-RESOLUTION GRAPHICS WORKSTATIONS

Probably the greatest limitation of the widely available PCs for use in the core courses is their medium- to low-resolution graphics displays. Distributed parameter problems arise often in courses on transport processes, separations, and reactor design, and their solutions, in the form of streamlines, isotherms, lines of constant composition, *etc.*, can be plotted using software for two- and three-dimensional graphics. As this software becomes easier to use and more widely available, the limiting factor shifts to the resolution of the graphics display. Thus far, researchers have found it necessary to use the more expensive, and less widely available, high-resolution graphics workstations such as the Evans and Sutherland, MicroVAX II/GPX, Apollo, and Sun. However, these are becoming cheaper and consequently will be more available to undergraduate students. They are endowed with full 32 bit processors and speeds in the range of 1-10 MIPS, which reduce the computation times for finite-element analyses and graphical transformations.

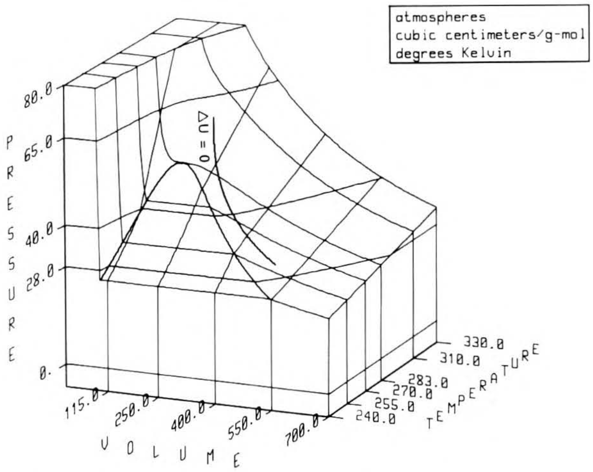

FIGURE 5. PVT surface for a van der Waals' fluid. Line of constant internal energy. (Reprinted with permission from [9])

An excellent example of the power of high-resolution displays is the program by Jolls [9] to plot three-dimensional PVT surfaces and related thermodynamic properties for the ideal gas and van der Waals' equations of state. The FORTRAN program, which runs on VAX computers with Tektronix 4107 color graphics terminals, is particularly effective in displaying the thermodynamic paths between two states. For example, isenthalpic, isentropic, isothermal, isobaric, *etc.*, paths can be displayed. See Figure 5, in which a path of constant internal energy is displayed on a PVT surface. While the Jolls displays are for pure fluids only, Gubbins and co-workers [10] have prepared composition-dependent displays for binary systems, as illustrated in Figure 6, using a FORTRAN program that runs on DEC VAX systems under VMS with Evans and Sutherland Multipicture System II workstations.

When similar workstations are mass-produced at lower costs, their impact on the teaching of subjects that benefit from three-dimensional visualization should be dramatic. For now, however, it seems reasonable to conclude that instructional computing lags behind current practice in several areas fundamental to classical chemical engineering, including thermodynamics and fluid mechanics.

LESS CONVENTIONAL PROCESSING

The processing of materials, biochemicals, biomedical systems, solar collectors, *etc.*, is often complex, difficult to model, and difficult to measure. As a consequence, until recently, young chemical engineers usually sought and found work in industries that apply the principles of transport processes, thermodynamics, chemical kinetics, *etc.*, to less complex processes. However, job opportunities are shifting toward the manufacture of silicon chips, the processing of pharmaceuticals and foods, the manufacture of solar collectors, *etc.*, and chemical engineers are being challenged to develop new sensing devices that provide better data and more detailed models to clarify their processing mechanisms.

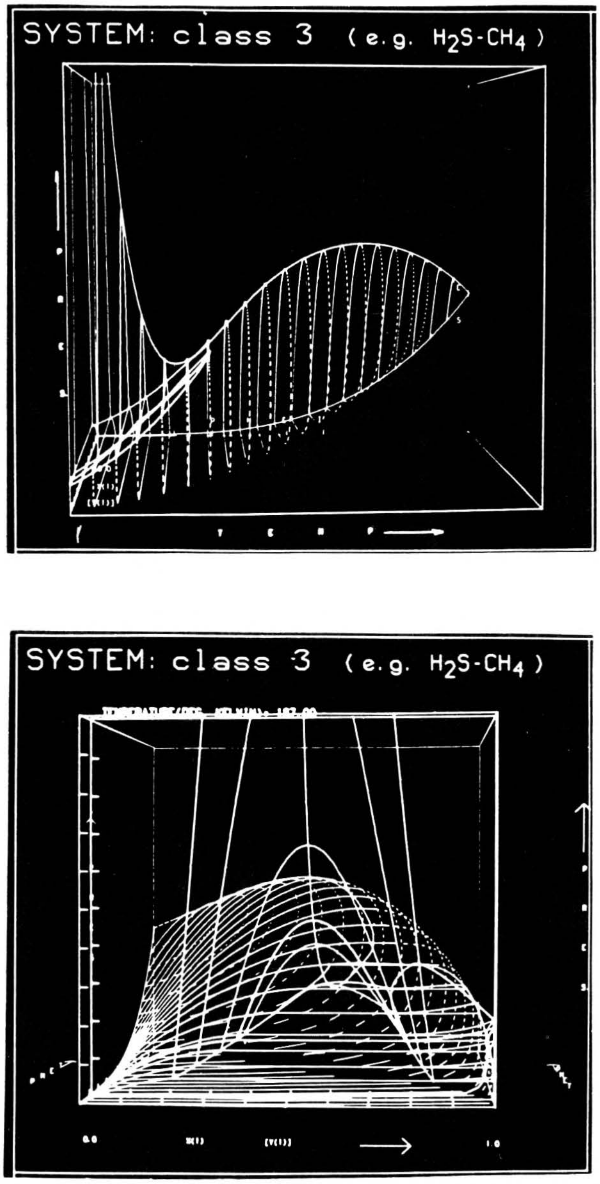

FIGURE 6. PTX surface for $H_2S - CH_4$ system using the Soave-Redlich-Kwong equation. (Reprinted with permission from [10])

Academicians are prominent in these fields and, consequently, are introducing new experimental and theoretical techniques as applications in their core courses and in specialized electives. With these areas expanding, it seems reasonable to question whether the computer is enabling undergraduate students to better understand, and possibly design, less conventional processes. The response, it seems clear, is *no;* or at least, *not yet.*

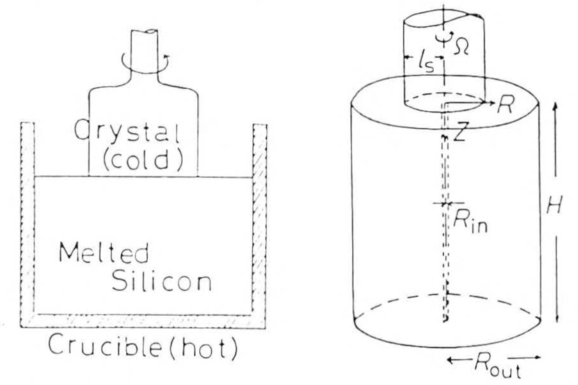

FIGURE 7. Three-dimensional modeling of Czochralski crystal growth in the manufacture of silicon chips [12].

The theoretical work of these researchers has become so computer-dependent that undergraduate students can be expected to gain exposure to their models as they evolve. In many cases, although the details of the models and finite-element analyses are beyond their comprehension, the students should be able to perform meaningful computational experiments, trying different geometries and configurations, calculating power requirements, *etc.* For the most part, these teaching materials will require high-resolution graphical displays with acceptable computing speeds and sufficient storage to perform the finite-element analyses.

One such application involves the Czochralski method of crystal growth in the manufacture of silicon chips [11], for which Ozoe and Matsui [12] have developed a three-dimensional model of the crucible shown in Figure 7. Their model accounts for the bouyant and centrifugal forces, with zero gradients assumed in the azimuthal direction, and confirms that at critical Raleigh numbers and critical ratios of

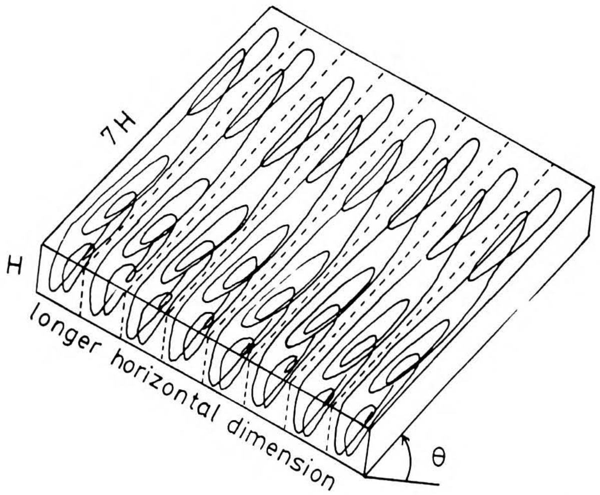

FIGURE 8. Sketch of the streaklines from three-dimensional modeling of natural convection in a solar collector [13].

Grashof number to Reynolds number squared, undesirable recirculation patterns develop in the crystalline melt. A related example involves natural convection in a solar collector that absorbs solar energy at the lower surface and transmits it to the fluid by convection and conduction. Figure 8 shows the system under study by Churchill and co-workers [13]. Their results show a three-dimensional transition in the pattern of flow and the rate of heat transfer as the angle θ varies. Clearly, programs that solve the partial differential equations and display the results in three dimensions can add immeasurably to courses in heat and mass transfer. At this time, the use of these programs for instructional computing lags far behind the development of these algorithms. The gap, however, can be expected to narrow appreciably over the next 2-3 years, as high-resolution graphical workstations replace the current generation of PCs.

CONCLUSIONS

It is concluded that:

- ***For the design and control courses, the computing tools are, for the most part, in step with design and control practice in chemical engineering. (See Part 1.)***
- ***Microcomputers are beginning to stimulate the use of open-ended problems in the core courses. The cost of software development, principally in student and faculty time, continues to be high. But, the new authoring systems have the potential to reduce the cost and associated effort sharply.***
- ***When high-resolution workstations are mass-produced at lower costs, their impact on the teaching of subjects that benefit from three-dimensional visualization should be dramatic. Currently, however, instructional computing lags behind the current practice in several areas fundamental to classical chemical engineering, including thermodynamics and fluid mechanics.***
- ***Complex computer models, often developed as a consequence of improved sensing devices, permit chemical engineers to clarify the mechanisms that underlie the processing of materials and biochemicals, the behavior of biomedical systems,*** etc. ***At this time, the use of such models for instructional computing lags far behind the development of models for these processes. The gap, however, can be expected to narrow over the next 2-3 years, as high-resolution graphical workstations replace the current generation of PCs.***

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