ChE curriculum

CHEMICAL ENGINEERING AND INSTRUCTIONAL COMPUTING*

Are They in Step?

PART 1

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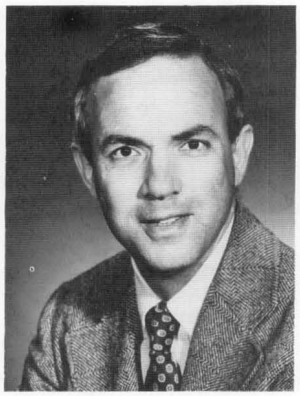
During the past five years, a large fraction of our chemical engineering graduates have found jobs in industries that utilize the principles of the transport processes, thermodynamics, and chemical kinetics, but whose primary operations are peripheral to the mainstream curriculum in chemical engineering and to the focus of the traditional chemical industries. These operations include biochemical and biomedical processing, advanced materials processing, solid-state electronics, and risk and hazard management. As a consequence, there have been calls for an enrichment of the chemical engineering curriculum with subject matter relevant to these fields by inclusion of applications in the common core courses and the development of new, specialized, elective courses. See, for example, the Proceedings of the Conference on "Chemical Engineering in a Changing Environment" [1] and the Amundson report [2].



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Concurrently, computers comparable in power to the mainframe processors of the mid-1960s (*e.g.*, the IBM 7090) have become inexpensive and highly interactive, and are now an integral part of our homes, offices, and laboratories. The rapid growth of this vast market has stimulated the development of high-quality, general-purpose software to permit data-base management, spreadsheet analysis, display of 2- and 3-dimensional colored graphics, numerical analysis, symbolic manipulation, and word processing. More specifically, in the chemical engineering curriculum, these systems, together with specialized packages for the synthesis and analysis of process flowsheets and control structures, the estimation of costs, *etc.*, have become widely used. Software for illustration of the concepts of transport processes, thermodynamics, and chemical kinetics, as well as those that emphasize biochemical and materials processing, has been slower to develop. In an effort to understand this situation, perhaps it is appropriate to trace the evolution and status of software for instructional purposes and to raise the question: "Chemical Engineering and Instructional Computing—Are They in Step?"

Initial efforts to use digital computation in chemical engineering coursework were unquestionably oriented toward the design course, followed closely by the process dynamics and controls course. With the advent of personal computers in the early 1980s, many more faculty became computer users and, al-

though there is some evidence of computer-oriented problems in courses other than design and control (*i.e.*, in courses on transport processes, thermodynamics, chemical kinetics, *etc.*), the level of utilization lags far behind that in the design and control courses.

This article is being published in two parts. Part 1 focuses on the design and control courses, whereas Part 2 (to be published in the next issue of CEE) concentrates on courses other than design and control.

DESIGN COURSE

One of the most significant developments in the field of process design has been the rapid evolution (in less than three decades) and widespread utilization of computing systems for the evaluation of alternative flow sheets. In the 1960s, many systems such as PACER [3] and CHESS [4] were introduced to perform material and energy balances and estimate equipment sizes and costs. Then, in 1973, the CACHE Corporation began facilitating the use of Monsanto's FLOWTRAN system over a communications network by many chemical engineering departments [5]. These first and second generation systems contained a library of subroutines to simulate the more conventional processing units, such as flash vessels, distillation towers, absorbers and strippers, liquid-liquid extractors, heat exchangers, compressors and turbines. For the most part, phase equilibrium was assumed in the separations, overall heat transfer coefficients were specified for the heat exchangers, and isentropic efficiencies characterized the compressors and turbines. Simple reactor models permitted the specification of the fractional conversions of key species or the extents of key reactions. All of the models were evaluated in the steady-state and the systems placed emphasis on the convergence of the recycle and control loops that typically arise through design specifications.

To permit generality in the modeling of streams with arbitrary mixtures of chemicals over broad ranges of temperature and pressure, physical property data banks were developed. In FLOWTRAN, the INF program implemented one of the first information systems to store and retrieve the physical constants for large numbers of chemical species in public and private files on random access disks. These systems permitted the engineer to select the data records and methods for estimating thermophysical properties such as the vapor pressure, density, enthalpy, and entropy of chemical mixtures. These facilities for selecting from amongst many subroutines and data were, in many respects, the precursors of today's *expert systems*.

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By 1985, with the advent of individual minicomputers for departments and engineering schools, FLOWTRAN had been installed in about 100 departments of chemical engineering. Concurrently, other commercial packages were widely installed, primarily PROCESS (Simulation Sciences) [6], DESIGN II (ChemShare) [7], and ASPEN PLUS (Aspen Tech) [8]. These are large systems, which are executed in batch mode and which require computing power greatly in excess of that provided by personal computers such as the IBM PC.

Each of these systems introduced special features, only a few of which can be mentioned here. ASPEN PLUS was the first to similate solids-handling equipment, including cyclone separators, flash driers, and crushers, with several models that account for heat and mass transfer between phases. Its reactor models implement nth-order kinetic expressions for CSTR and PFTR configurations. DESIGN II utilizes a stand-alone package, CHEMTRAN, for the estimation of thermophysical properties. Its data base contains the physical constants (T_c, P_c, T_{NBP}, . . .) for nearly 1000 chemicals. Probably the most important characteristic as far as use by undergraduates in their design projects is concerned, is the ability of this package to estimate the physical constants for organic molecules using group- and bond-contribution methods. At the University of Pennsylvania, with a separate design project for each group of three seniors, unusual chemicals are often encountered. It is difficult to locate physical property constants for some of these chemicals, and CHEMTRAN enables the students to begin their design calculations while they continue their search for data. In addition to the physical constants for some of these chemicals, CHEMTRAN estimates activity coefficients using the UNIFAC group-contribution method. Hence, it can estimate the properties of nonideal mixtures of organic molecules even when *no* physical property data are available.

In the past five years, these systems have been augmented to permit the optimization of process flow sheets subject to equality and inequality constraints specified by the engineer. For example, Biegler [5] added the successive quadratic programming algorithm, QPSOL, to FLOWTRAN. His interface,

SCOPT, and the QPSOL algorithm are distributed by the CACHE Corporation.

Also, during this period, with the availability of PCs, COADE prepared a microcomputer version of CHESS called MICROCHESS and recently upgraded it to CHEMCAD [9], a highly interactive package which displays process flowsheets as illustrated in Figure 1. A similar package is HYSIM [10] by Hyprotech, Ltd. These packages are finding widespread usage in the chemical engineering curriculum. Two other packages that run on an IBM PC with an IBM 370 board are ChemShare's DESIGN II and ASPEN/SP-PC [11], but these are not being used by any academic departments, to my knowledge.

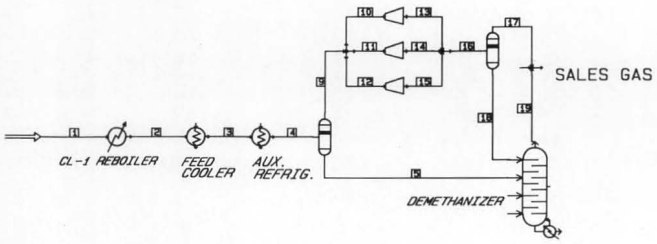


FIGURE 1. CHEMCAD [9] flowsheet for design of a gas plant.

It is noteworthy that stand-alone, microcomputer packages are becoming useful for the undergraduate design courses. One, in particular, is the CHEMCOST [12] program by COADE. CHEMCOST provides up-to-date estimates for the capital cost of the individual process units in a chemical plant.

Software systems for the synthesis of process flowsheets have been less successful than those for analysis, with the exception of software for the synthesis of networks of heat exchangers. Union Carbide's ADVENT system [30] provides excellent color graphics displays of the process flow sheets and the heat integration diagrams that result from the implementation of Linnhoff's Temperature Interval Method [13]. Although the ADVENT System is not available to universities, the Linnhoff March Co. recently began distributing, through the CACHE Corporation, a less complete system, TARGET II [31], that runs on the IBM PC. TARGET II determines the minimum requirements for hot and cold utilities, but does not match the hot and cold streams to synthesize a network of heat exchangers. A more complete system, called HENS [14], has been prepared for the AT&T 6300 microcomputer. HENS enables the student to position heat exchangers on a heat integration diagram interactively. To my knowledge, however, it is not being widely used. Other packages, with automated facilities to design the networks of heat exchangers, but not implemented on microcomputers with highly-interactive graphics, are HEXTRAN (Simulation Sciences) [15], RESHEX [16], and MAGNETS [17].

PROCESS CONTROL

In process control, mainframe packages have never achieved the popularity of the comprehensive packages developed for the analysis of the flow sheet in process design. One such package, ACS [18], developed to run on the IBM 4341, performs the dynamic simulation of processes with alternate control structures (*e.g.*, PID, lag/lead, ratio, cascade, . . .). It has been used in the control courses of approximately fifteen chemical engineering departments.

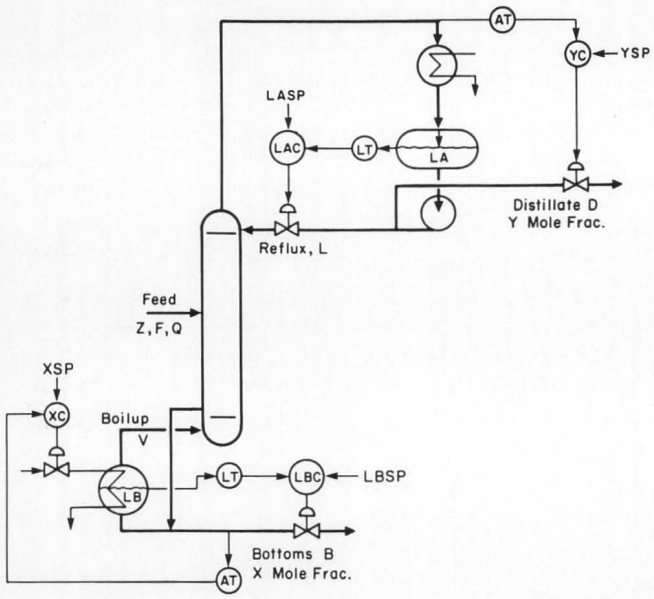
In the area of digital control, more emphasis has been placed on real-time interaction, initially with minicomputers and more recently with microcomputers. Many control laboratories have been created using microcomputers, as exemplified at Washington University [19].

Traditionally, procedures for the design of process control systems have involved the analysis of linearized systems in the Laplace and frequency domains. With the recent generation of microcomputers, system designers have added highly interactive graphical interfaces that display Bodé and Nyquist plots, Root-Locus diagrams, responses in the time domain, *etc.* One such package, CC (Systems Technology Corp.) [20], runs on the IBM PC and is used at many universities. It includes facilities to convert between the state-space and the Laplace and Z-domains, and to implement optimal control algorithms. A more complete package, CONSYD [21], is available for VAX computers, but provides a lesser quality of graphical interaction. Yet, another package, PROCOSP [22], provides better interactive graphics on the IBM PC with a *mouse*. PROCOSP focuses on the design of PID controllers that satisfy the engineer's specifications for the overshoot ratio and settling time.

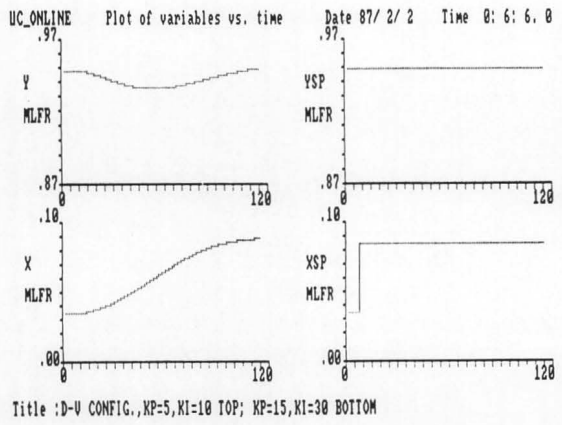
Of course, many chemical processes are highly nonlinear. Hence, software systems that permit both the steady-state and dynamic simulation of alternate control structures can be very helpful. For the analysis of process flowsheets, probably the SPEED-UP system [23] has received the most publicity in recent years. This package has been used successfully in industry and is expected to be distributed by the CACHE Corp. to the universities in the near future. SPEED-UP has not been installed on PCs and, consequently, can be expected to have limited facilities for graphical interaction.

A more specialized package is UC ONLINE [24] for the simulation of distillation towers with alternate multiloop PID feedback control schemes. UC ONLINE runs on the IBM PC with interactive graphics. For example, the distillation tower and control structure displayed in Figure 2a were simulated after a step-change in x_{sp}, with the response plotted in Figure 2b. UC ONLINE has been distributed to several university departments.

Before long, it can be expected that packages for the bifurcation analysis of nonlinear systems, both steady-state and dynamic, will be used routinely for studying their performance and stability [25]. Programs for bifurcation analysis, such as AUTO [26], should become widely used.



(a) P&ID



(b) Response to a step-change in x_{sp}

FIGURE 2. Distillation control with UC ONLINE [24].
(Reprinted from *CEE*, **21**, 122-123.)

EXPERT SYSTEMS

The current flurry of activity to develop logic-based systems has been confined principally to the design and control areas. One such expert system was created by Shinskey [27] to design multiloop control systems for distillation towers. It was written in BASICA to be run on an IBM PC. Given specifications for a tower, controlled and manipulated variables, Shinskey's system calculates relative gains and selects the control structure by threading through decision trees with approximately 1000 rules, before drawing the PID. Other expert systems are being developed to detect faults in chemical plants [28] and to estimate thermophysical properties by selecting an appropriate combination of estimation methods [29].

It is especially noteworthy that, as of this writing, there is no evidence of the use of expert systems in chemical engineering coursework. A Task Force of the CACHE Corporation is working to prepare monographs that show how to apply the principles of artificial intelligence in building expert systems.

PARTIAL SUMMARY

Having traced the evolution of instructional computing in the design and control courses, it seems reasonable to conclude that the computing tools for undergraduate instruction are, for the most part, in step with design and control practice in chemical engineering. In some cases, the computing systems used by undergraduate students are less elaborate than those available to industrial practitioners. In other cases, the tools are those that have evolved in university research and are more advanced than those used in industry.

The successes in the design and control areas have, for less well-understood reasons, not been paralleled in the courses that focus on the transport processes, thermodynamics, and chemical kinetics. This has led the Curriculum Task Force of the CACHE Corporation to seek answers to two questions:

- ***Can microcomputers stimulate the use of "open-ended," design-oriented problems in these courses?***
- ***Can high-resolution displays permit students to better learn the principles through visualization of streamlines in fluid flows, visualization of PVT surfaces, etc.?***

These questions, together with one other:

- ***Can computers enable undergraduate 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.?

will be addressed in Part 2 of this paper, to be published in the fall 1988 issue of *CEE*. □

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ChE book reviews

HANDBOOK OF SEPARATION PROCESS TECHNOLOGY

Edited by R. W. Rousseau
John Wiley & Sons, Inc., 1530 S. Redwood Rd., Salt Lake City, UT 84104; $69.95 (1987)

Reviewed by
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Webster's *Third New International Dictionary* defines "Handbook" as

1. A book capable of being conveniently carried as a ready reference.
2. A concise reference book covering a particular subject or field of knowledge.

For an engineering handbook, this writer would add: For the engineer facing a plant problem, a handbook

1. Provides sufficient information on theory and application to enable equipment selection.
2. Details the information required for equipment sizing.
3. Provides infomation necessary for estimating equipment and operating costs.