ChE classroom

THE PROCESS DESIGN COURSES AT PENNSYLVANIA:* Impact Of Process Simulators

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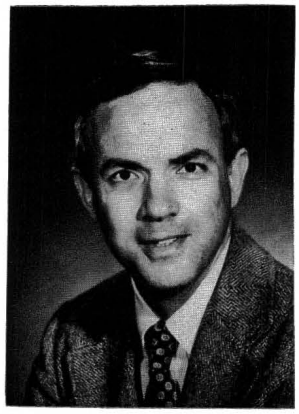
FOR THE PAST 35 years, a two-semester process design sequence has been taught at the University of Pennsylvania. This sequence is unique in several aspects, most notably its diversity of design projects, involving seven faculty advisors and seven consultants from local industry. The fall lecture course, "Introduction to Process Design," covers the methodology of process design and prepares our students for the spring project course, "Plant Design Project," which is intended to provide a meaningful design experience. This article is focused on the impact of process simulators in recent years.

In 1967, we began to introduce computing technology and modern design strategies, principally in the sophomore course on "Material and Energy Balances," and have gradually integrated process simulators into the design sequence. Our objective was to strengthen the highly successful sequence developed by Melvin C. Molstad, A. Norman Hixson, other faculty, and our many industrial consultants. From 1967-1973, our efforts to develop educational materials (principally software) far outweighed the benefits to the students. However, in 1974, the availability of Monsanto's FLOWTRAN Simulator finally made this step successful. Additional industrial simulators have since become available and the benefits to our students now far outweigh our past efforts.

*Based on a lecture at the ASEE Summer School for ChE faculty, Santa Barbara, CA, August, 1982.

Initially, the steps to satisfy a societal need are summarized e.g., the conversion of coal to liquid and gaseous fuels.



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Design courses are normally taught last in the chemical engineering curriculum and, hence, the details of the lecture course depend somewhat on the prerequisite courses—and class size. Hopefully, this discussion of our particular format will provide useful ideas.

FALL LECTURE COURSE: INTRODUCTION TO PROCESS DESIGN

The outline of topics and associated lecture hours are listed in Table 1. Two books are required: *Plant Design and Economics for Chemical Engineers* [7], and *FLOWTRAN Simulation—An*

TABLE 1
Outline of topics. Fall lecture course.

	Lecture Hours
Introduction	1
Process Synthesis	1
Analysis of Flowsheets—FLOWTRAN Simulation	12
Design of Heat Exchangers	8
Cost Estimation	3
Time-Value of Money, Taxes, Depreciation	3
Profitability Analysis	2
Optimization	3
Heat Integration	4
Synthesis of Separation Processes	2
Selection of Design Projects (for Spring Project Course)	1
Exams	2
	42

Introduction [9]. In addition, materials are taken from seven other sources which are placed on reserve in our library [1, 2, 3, 4, 5, 6, 11].

The course expands upon the steps in the development of a new chemical process as shown in Fig. 1 (based upon a similar figure in Rudd and Watson [8]). Initially, the steps to satisfy a societal need are summarized; e.g., the conversion of coal to liquid and gaseous fuels. Of course, the steps are not always carried out in the sequence shown. For example, a sensitivity analysis is often performed prior to an economic analysis. In the integrated plants of today, aspects of transient and safety analysis must also be considered in the synthesis of the process flowsheet.

Next, the steps in the synthesis of a vinyl chloride process are illustrated with the intent of exposing the steps that enter into the invention of alternative flowsheets. Fig. 2 shows the evolution of one flowsheet, beginning with selection of the reaction path (not shown), followed by the distribution of chemicals (matching sources and sinks and introducing recycle), selection of the separation steps, the temperature and phase change operations (not shown), and, finally, the integration into chemical process equipment. This is based upon Chapter 3, "Process Synthesis," in *Introduction to Chemical Engineering and Computer Calculations* [6]. It is noteworthy that steam is used to vaporize dichloroethane and cooling water to cool the reaction products in a quench operation. We emphasize the desirability of heat integration, when feasible, but because carbon would deposit in the evaporator tubes, a rapid low-temperature quench, with water as the cooling medium, is necessary.

Principal emphasis is given to the subroutines to model the process units such as vapor-liquid separators, multi-staged towers, heat exchangers, compressors, and reactors.

Having introduced the concepts of flowsheet synthesis, attention is turned to the analysis of alternative flowsheets. In practice, of course, the two go hand-in-hand. FLOWTRAN is used principally because our book [9] is written in a tutorial fashion, as compared with the usual User Manuals. FLOWTRAN has been available for students on United Computing Systems, but its usage has been limited by the relatively high cost of commercial computers. Recently, however, like ChemShare (DESIGN/2000) and Simulation Sciences (PROCESS), Monsanto has made FLOWTRAN available for installation on university computers—

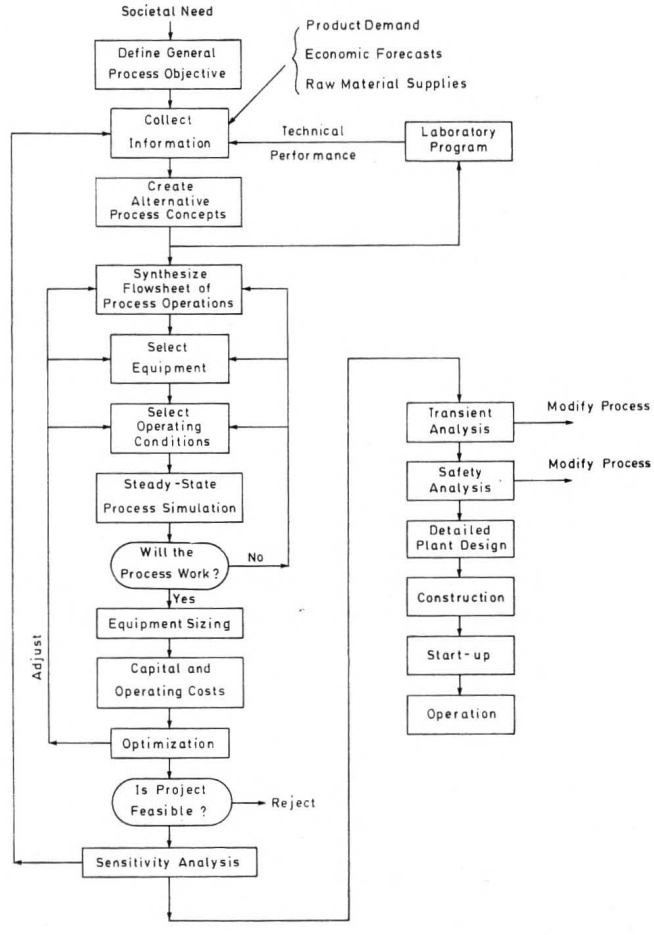


FIGURE 1. Steps in the development of a new chemical process.

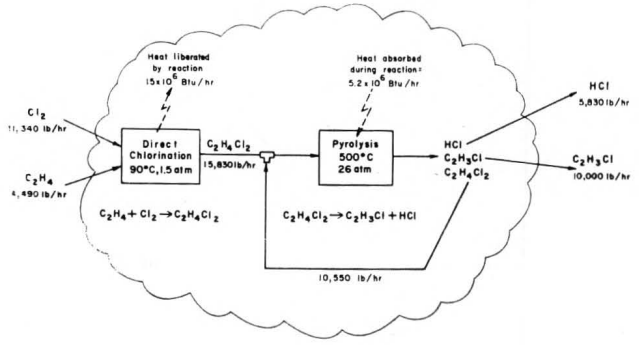
greatly improving the effectiveness of process simulators in the design course.

Principal emphasis is given to the subroutines to model the process units such as vapor-liquid separators, multi-staged towers, heat exchangers, compressors, and reactors. There are several subroutines to solve the equations that model each process unit. The models vary in specifications and rigor and it is important that the design student understand the underlying assumptions, but not the solution algorithm. We review the assumptions and make recommendations concerning usage of the subroutines listed in Fig. 3. For example, the PUMP routine disregards the capacity-head curve and uses the viscosity of *pure water*. When designing a distillation tower, use of DSTWU is recommended to calculate the minimum number of trays, the minimum reflux ratio, and the theoretical number of trays (given the reflux ratio), followed by DISTL which uses the Edmister assumptions to simulate the tower and, in some cases, FRAKB or AFRAC to solve the MESH equations with fewer assumptions.

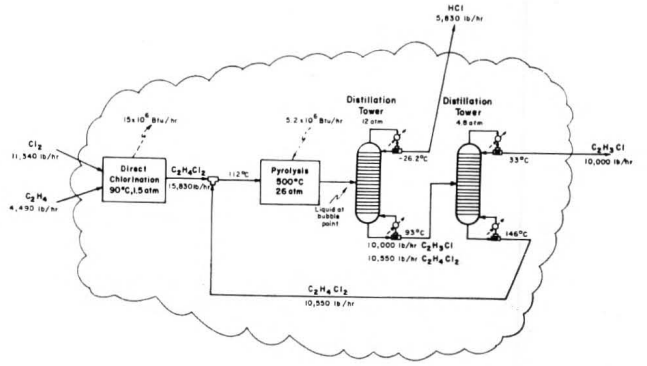
The synthesis of the simulation flowsheet is also emphasized with consideration of novel ways of using the subroutines to analyze a process flowsheet. For example, consider the quench process (Fig. 4a) in which hot gases are contacted with a cold liquid stream. Given the recycle fraction, and assuming that the vapor and liquid products are at equilibrium with no entrainment, most designers would develop the simulation flowsheet shown in Fig. 4b. However, iterative recycle calculations are unnecessary because the vapor and liquid products (S3, S5) are independent of the recirculation rate. In a more efficient simulation flowsheet, the IFLSH subroutine determines the flow rate and compositions of S3 and S5 (see Fig. 4c). Then, MULPY subroutines compute the flow rates for S4 and S6. Most students use the "brute-force" approach in Fig. 4b, requiring about 5-10 iterations with Wegstein's method, before we demonstrate that the iterative recycle calculations can be avoided.

These lessons are reinforced with a problem to simulate the reactor section of the toluene hydrodealkylation process [9, p. 228]. Feed toluene is mixed with recycle toluene and a recycle gas stream. The reaction products at 1268°F are quenched and the recycle fraction is adjusted to reduce the product temperature to 1150°F. As above, the iterative recycle calculations can be avoided, although most students use the brute-

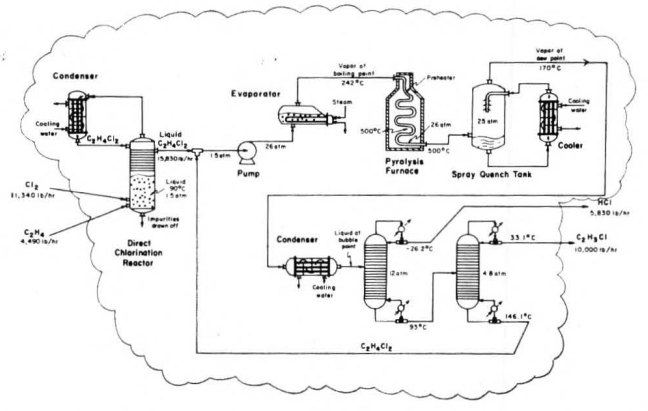
a) The process synthesis problem



b) Flow sheet showing distribution of chemicals for thermal cracking of dichloroethane from chlorination of ethylene (reaction past 3)



c) Flow sheet showing separation scheme for vinyl chloride process



d) Flow sheet showing task integration for the vinyl chloride process

FIGURE 2. Synthesis of a vinyl chloride process (Myers and Seider [6]).

force approach.

The FLOWTRAN subroutine EXCH1 implements the method of thermodynamic effectiveness (computes terminal temperatures, given the area and overall heat transfer coefficient), and the EXCH3 subroutine implements the log-mean temperature difference method (computes the area, given terminal temperatures and overall heat transfer coefficient). Since these methods are not covered in our course on heat and mass transfer, the methods are derived and problems are worked using Chapter 11 of *Principles of Heat Transfer* [5] as text material. Then, the students design a heat exchanger (e.g., 1-4 parallel-counterflow) with correlations for the heat transfer coefficients and pressure drops on the shell and tube sides and the methods presented by Kern [4] and Peters and Timmerhaus [7]. This exposes the student to more detailed analysis procedures than are available in most process simulators. Such detail is recommended only when the approximate models introduce large errors and the cost of a heat exchanger contributes significantly to the economics of the process.

This leads to methods of cost estimation. FLOWTRAN has subroutines for cost estimation, but the assumptions of the cost models are not stated or referenced. Since no basis is available for justifying their results, well-established and clearly stated methods are preferred. The factored cost methods of Guthrie [3] have been used to date, but the factors in his article need updating. We are evaluating the PCOST program developed at Purdue University [10] and the data books of Woods [12]. Both give cost curves and factors based upon more recent cost data.

FIGURE 3
FLOWTRAN subroutines (blocks)

Flash	**IFLSH**	**Isothermal flash**
	AFLSH	**Adiabatic flash**
	BFLSH	**General purpose flash**
Stagewise separation	**SEPR**	**Split fraction specification**
	DSTWU	**Winn-Underwood-Gilliland distillation**
	DISTL	**Edmister distillation**
	FRAKB	**Tray-to-tray distillation (KB method)**
	AFRAC	**Tray-to-tray distillation and absorption (matrix method)**
Heat exchange	**HEATR**	**Heat requirement**
	EXCH1	**Shell and tube—method of thermodynamic effectiveness**
	EXCH3	**Shell and tube—log-mean temp. diff. method**
Reactor	**REACT**	**Fractional conversion specification**
	XTNT	**Extent of reaction specification**
Compression	**PUMP**	**Centrifugal pump**
	GCOMP	**Compressor (or turbine)**
Misc.	**ADD**	**Mixer**
	SPLIT	**Stream splitter**
	MULPY	**Stream multiplier**

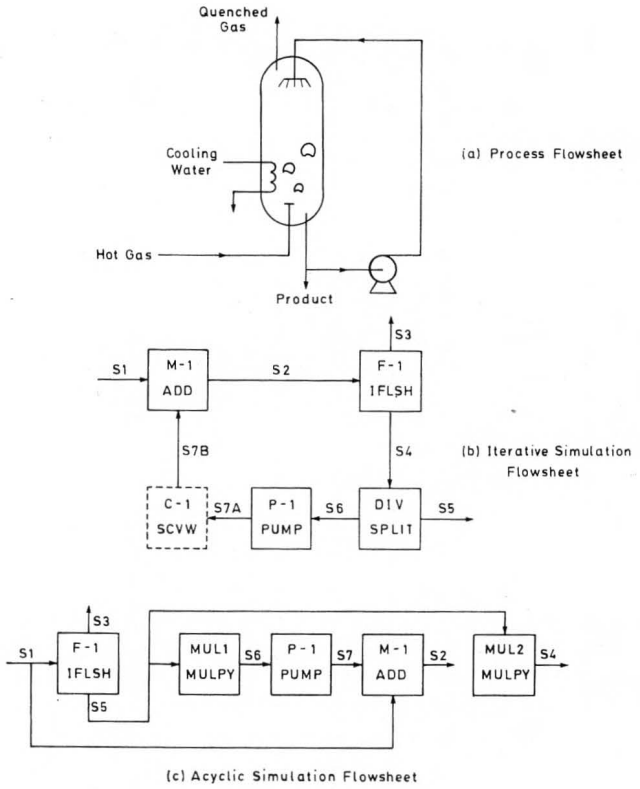


FIGURE 4. QUENCH process.

For production or operating costs, the recommendations of Peters and Timmerhaus in Chap. 5 are used with concentration on the direct production costs, such as for raw materials, operating labor, and utilities. The Chemical Marketing Reporter provides the costs of chemicals bi-weekly (often for several locations within the United States).

Next, the concepts of profitability analysis are introduced, following the sequence of Peters and Timmerhaus in Chaps. 6-9. The concepts of simple and compound interest are applied to give the present and future values of an investment and to define an annuity. Then, capitalized costs are covered to provide a basis for evaluating the cost of equipment having different service lives. For

Continued on page 41.

The liquid water product comes from open steam used to assist in the first crude oil fractionation instead of having a reboiler.

GENERAL FRACTIONATION NOTES

(a) The optimum reflux ratio is said by Treybal to fall in the range of 1.2 to 1.5 times the minimum reflux ratio. This rule was formulated when heat was cheap, say \$0.50 to \$1.00 per million Btu. With currently expensive heat, say \$5.00 to \$8.00 per million Btu the optimum reflux ratio comes much nearer to the minimum and may lie in the range (1.05 to 1.2) (R_{min}).

(b) In desert areas when water is scarce and expensive, air cooling is often used to condense the overhead vapors but in this case the overall heat transfer coefficients are much lower than with water cooling and the optimum approach temperature differences for condensing may be much larger than the 10° to 20°F quoted above. Also the design air inlet temperatures may have to be 90° to 110°F or even 120°F in order to get a design which will work most of the time. □

DESIGN COURSE

Continued from page 29.

projects with gross profit, tax and depreciation schedules are described. Finally, cash flow diagrams are introduced for comparing investments on the basis of simple rate of return, present worth of cash flows, or discounted cash flows.

Given profitability measures, questions of optimality arise. The optimization problem is defined in general terms to begin coverage of this comprehensive subject. The objective is to introduce optimization methods, suggesting the need for further study. Single variable, unconstrained methods known as sequential search methods (e.g., the Golden-Section method) are covered using the excellent descriptions in Chap. 10 of *Digital Computers and Numerical Methods* [2] with two example problems from Chap. 10 of Peters and Timmerhaus (optimal insulation thickness and optimal batch time). Then, multivariable, unconstrained methods are covered including lattice search, repeated uni-directional search, and optimal steepest descent [2].

Next, the students optimize the design of a distillation tower with a condenser, reboiler, and reflux pump. Throughout the course they have solved problems involving these components, so for this problem they are given the FORTRAN function DISTIL which computes the rate of return on investment as a function of the product purity, the reflux ratio, and the fractional recovery of the most volatile species in the distillate. The use of DISTIL to (1) carry out material balances, (2) count trays, (3) calculate the tower diameter, heat exchanger areas, and pump horsepower, and (4) calculate costs, cash flows and discounted cash flow rate of return is reviewed. Then, the students write a program to calculate the maximum rate of return on investment. Incidentally, DISTIL was written by Prof. D. Brutvan [1] and has been modified slightly for use in our course. Prof. Brutvan prepared an excellent problem-statement, typical of a large company, with design specifications, sources of physical property data, cost data, and explanations of the algorithm. This has also been modified for use in our course.

After the introduction to process synthesis, the course concentrates on analysis with the configuration of the process flowsheet given. The design variables are adjusted to locate an optimal design for a given configuration. However, in process synthesis, the emphasis is placed upon finding the best configuration. This approach is well-suited to teach methods of increasing the thermodynamic efficiency by heat integration. The monograph, *Availability* (*Exergy*) *Analysis* [13] and the paper "Heat Recovery Networks" [11] provide excellent introductions to the analysis of thermodynamic efficiency and the pinch method for minimizing utilities. Synthesis of separation processes is also covered, but briefly in just two hours. The key considerations are introduced, time being unavailable to solve a meaningful problem.

The course concludes with a final exam and the course grade is based upon two mid-semester exams and the homework. Approximately 15 problem sets are assigned, with two problems using FLOWTRAN and one problem in which the rate of return for a distillation tower(using the DISTIL function) is maximized.

SPRING COURSE: PLANT DESIGN PROJECT

Penn's strength in process design can be attributed in part to the large concentration of chemical industry along the Delaware River and to our close interactions with several industrial

colleagues. In this section, organization of the project course to benefit from this interaction is examined, before considering the impact of process simulators.

During the last two weeks of the fall lecture course, the students select design projects suggested by our industrial colleagues and the chemical engineering faculty. The projects must be timely, of practical interest to the CPI, and be workable in 15 weeks. Kinetic and thermophysical property data should be available. Abstracts of possible design projects are prepared and the students select a project or propose one of special interest to themselves. No effort is made to restrict projects to those well-suited for simulation.

In the spring, 1982, we had sixteen projects, one for each group of three students, and in 1983 we had nineteen projects. Each group is advised by one of seven members of our faculty, usually supplemented by a visiting faculty member and a research student in the area of computer-aided design.

During the spring, as the designs proceed, each group meets for one hour weekly (on Tuesday afternoon) with its faculty advisor and one of its four industrial "consultants." For the past three years we have had seven outstanding consultants. Dr. Arnold Kivnick of Pennwalt Corp. has completed his twenty-fifth year as a consultant to our students. Arnold has shared his years of experience in helping our students and young faculty develop their design skills. Other members of our consultant team contribute similarly, making it possible to expose our students to a broad range of design projects.

The course concludes with a one-day technical meeting of oral presentations accompanied by written design reports. From the oral and written reports, the faculty selects the outstanding design project for the Melvin C. Molstad Award. Each member of the winning group receives a $100 prize thanks to the generous endowment of Dr. Ken Chan, Class of 1962. Notably, the last five reports have also won the Zeisberg Award in competition with other schools in our area.

A typical abstract of a design project is shown in Fig. 5 and the titles for 1982-83 are in Table 2. The problems are timely and their diversity shows the broad interests of our faculty and industrial consultants.

FIGURE 5
Abstract of a typical design project

High purity isobutene
(suggested by Len Fabiano, ARCO)

Isobutene will be recovered from a mixed C_4 stream containing n-butane, i-butane, butene-1, butene-2, i-butene, and butadiene. A four-step sequence will be considered: (1) reaction with CH_3OH to MTBE (methyl-tertiary-butyl-ether), (2) recovery of MTBE from the reaction products, (3) cracking of MTBE to methanol, isobutene, and by-products, and (4) recovery of isobutene, by-products and methanol.

This design will concentrate on (3) and (4). Kinetic data in the literature will be supplemented by ARCO.

Fattore, Massi Mauri, Oriani, Paret, "Crack MTBE for Isobutylene," Hydrocarbon Processing, 101, Aug., 1981.

TABLE 2
Possible Design Projects (1982-83)

		Suggested by
1.	Cyclohexane oxidation to cyclohexanol	W. D. Seider
2.	Polymerizer solvent recovery	D. F. Kelley, DuPont
3.	High purity isobutene	L. A. Fabiano, ARCO
4.	Catalyst recovery plant	L. A. Fabiano, ARCO
5.	Triolefin process	L. A. Fabiano, ARCO
6.	Ethylene dimerization	L. A. Fabiano, ARCO
7.	Ethanol to gasoline	W. B. Retallick, Cons.
8.	Methane from coal with K_2CO_3 catalyst	W. D. Seider
9.	Liquid CO_2 for extraction of pyrethrin from chrysanthemums	W. D. Seider
10.	Syngas to methanol	S. W. Churchill
11.	Separation of benzene, toluene, xylene	W. D. Seider
12.	Heat pump for ethane-ethylene split	W. D. Seider
13.	Optimization of solar heated home	N. Lior
14.	Maleic anhydride from butane	W. D. Seider
15.	Fluidized-bed, coal combustion, electric power plant	N. Arai
16.	Supercritical fluid extraction	A. L. Myers
17.	Dimethylamine	P. J. O'Flynn
18.	Paramethylstyrene with zeolite catalyst	W. D. Seider
19.	Hydrogen production by radiation of CO_2 and water-gas shift	S. W. Churchill

IMPACT OF SIMULATORS

Since 1974 we have had access to the FLOWTRAN program on United Computing Systems (UCS), but its usage has been limited by the high cost of UCS, a commercial computing system. Initially modest funds were budgeted for FLOWTRAN, but with increasing class sizes and tight budgets it became necessary to charge the

students for use of FLOWTRAN. Consequently, FLOWTRAN was used by just a few groups —as a last resort. The maximum charge per group was approximately $100.

In 1982, ChemShare Corp. provided DESIGN/2000 as a load module for installation on our UNIVAC/1100 at no cost to the University of Pennsylvania. Subsequently, eight of the sixteen design groups chose to use DESIGN/2000, averaging $800 of computer charges per group.

DESIGN/2000 has a well-developed thermophysical property system, CHEMTRAN, with a data bank containing constants for 900 chemicals (as compared with 180 in the student version of FLOWTRAN). Programs are available to calculate constants such as the normal boiling point temperature and critical properties, given the molecular structure (the atom-bond interconnections). For nonideal solutions, programs are available to compute the interaction coefficients for the UNIQUAC equation and, when equilibrium data are unavailable, to estimate activity coefficients using the UNIFAC group interaction coefficients. Furthermore, CHEMTRAN provides the Soave-Redlich-Kwong and Peng-Robinson equations for calculations in the vapor-liquid critical region. In addition to these advantages (compared with FLOWTRAN), alternative programs are provided for short-cut and rigorous analysis of multistaged towers.

Similarly, the PROCESS system of Simulation Sciences, Inc., provides features that are not included in the student version of FLOWTRAN. Some are equivalent to DESIGN/2000, some are not in DESIGN/2000, while some of the DESIGN/2000 features are not included. PROCESS has not yet been installed on our computer, so that we are less familiar with this system.

Several limitations remain and these are gradually being eliminated. However, currently FLOWTRAN, DESIGN/2000 and PROCESS do not model processes with inorganic compounds and ionic species. There are no programs to calculate compositions in phase and chemical equilibrium or to simulate CSTRs, PFTRs, and solids-handling equipment. These features have been included in the ASPEN system, but ASPEN is not yet available for routine student usage. As expected, ChemShare and Simulation Sciences are adding many of the same features.

The bottom line with respect to our design sequence is that industrial process simulators permit more routine analysis of simple processes and give more accurate analyses for complex precesses; for example, extractive distillation towers. These simulators enable more complete parametric analysis and examination of process alternatives. Normally, they are applicable for just parts of the analysis; rarely for analysis of the entire flowsheet. They provide our students with experience in the use of modern CAD tools.

In our research, the development of new CAD methodologies is emphasized. In the senior design course, some of these methodologies are introduced using well-tested industrial simulators which are gradually upgraded. Emphasis is placed on completing the design. Student time is not wasted working out difficulties with a prototype program.

When possible, process synthesis methodologies are emphasized. As yet, however, few projects have been found which are sufficiently open-ended to permit analysis of many alternate configurations in the fifteen week term. Good suggestions are welcomed. □

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