AN ELECTIVE COURSE ON COMPUTER-AIDED PROCESS DESIGN

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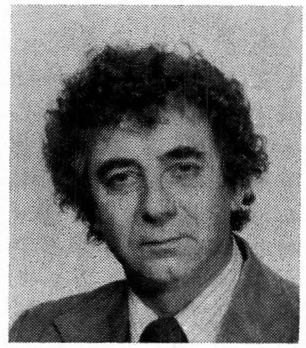
THE SCHOOL OF CHEMICAL Engineering at Georgia Tech is one of the largest in the country and, over the past five years, has granted around 70-80 undergraduate degrees annually. Hence, there is the opportunity, as well as the demand, for a variety of undergraduate elective courses. Many of these elective courses are offered as an integral part of the design program, which has been described elsewhere [1]. By way of example, presentations have been made of the elective courses on pulp and paper technology [2] and on project engineering [3]. A paper was also presented several years ago, which described early experiences with an elective course on computer-aided process design [4]. The purpose of this article is to summarize additional experience since then, during which time there have been some interesting developments in this particular area of chemical engineering education.

COURSE OBJECTIVES

THIS COURSE ON computer-aided process design was first conceived in 1972 and offered in the spring quarter of 1973. Its purpose then and now is to familiarize the student with the synthesis and operation of large-scale computer systems for steady-state simulation of chemical processes as a design tool. This course is not a requirement in the undergraduate chemical engineering curriculum. Rather, it is an elective course intended for undergraduate students (senior level) who are interested in and likely to participate in process design, process engineering or process development work after graduation. By way of background, similar efforts in this area at other schools have been described, for example, by Gaddy [5] and by Westerberg [6].



Jude T. Sommerfeld has been a professor of ChE at Georgia Tech since 1970. He teaches courses on process control, distillation, reactor design and process design, and his research interests include energy conservation. He has also served as a consultant to numerous industrial organizations. Prior to 1970 he had eight years of engineering and management experience with the Monsanto Company and BASF-Wyandotte Corp. Dr. Sommerfeld received his B.Ch.E. degree from the University of Detroit, and his M.S.E. and Ph.D. degrees in chemical engineering from the University of Michigan.

The undergraduate program in chemical engineering at Georgia Tech has traditionally been very practice-oriented. More than 70% of the graduates from this program accept their first employment in industry. Less than 10% carry on to graduate studies in chemical engineering. Hence, this course on computer-aided process design, like most of the undergraduate chemical engineering curriculum, is of a very practical nature. Thus, the emphasis in this course is on the structure and usage of computer-aided design systems, with little or no sophisticated theory or mathematical developments.

COURSE STRUCTURE

MOST OF THE STUDENTS who elect this course do so in the final quarter of their senior year. Thus, they are often taking this course together with the required senior-level course on plant design, which has been found to be of some value. The amount and nature of the student enrollment in the computer-aided process design course over the past six years are summarized in Table I.

This elective course carries three quarter hours of credit, and the weekly schedule consists of two hours of lecture and one three-hour laboratory. The actual amount of course time devoted to the modelling of specific items of process equipment varies somewhat, depending upon the processes selected for study. The laboratory time is devoted to the development, debugging and discussion of computer programs.

There are two one-hour quizzes which are normally administered in this course. A tradition at Georgia Tech is that graduating seniors are exempt from all final examinations in their last quarter. Since the great majority of students who elect this computer-aided design course are graduating seniors, there is no final examination given in this course.

TABLE 1
Student Enrollment: Computer-Aided Process Design Course

Year (Sp. Quarter)	Student Enrollment Undergraduate	Graduate	Total
1973	13	4	17
1974	15	3	18
1975	11	3	14
1976	11	2	13
1977	17	6	23
1978	19	5	24

INSTRUCTIONAL MATERIALS

THE TEXT USED IN THIS course in its first two offerings was the book by Crowe and coauthors [7] on chemical plant simulation. Chapters 1-3 and 5 of this text were normally covered, irrespective of the particular processes studied. The selection of the remaining reading material from this text was somewhat dependent upon the processes selected for study. The students were generally satisfied with the selection of this textbook. The only regularly voiced criticism was that this text is too heavily oriented toward the description and application of a system (PACER) which was not easily available and hence not used in this course. A suggested improvement was more general discussion of computer-aided design systems (including physical property systems) and less examples of usage of the PACER system.

The year 1974 saw a major development in chemical engineering education. Successful negotiations between the CACHE (Computer Aids to Chemical Engineering) Corporation and the Monsanto Company resulted in the installation and maintenance of FLOWTRAN on a commercial network for use by chemical engineering educators. FLOWTRAN is a large, general-purpose simulator of chemical processes with extensive facilities for physical and thermodynamic property data handling and a large library of equipment modules, including cost estimation capability. It was developed by the Monsanto Company for internal use and was offered, for a time, as a commercial service by Monsanto. A cash grant was also provided by Monsanto to subsidize the installation of FLOWTRAN on the United Computing Systems, Inc. (UCS) commercial network and the preparation of a text [8] by the CACHE Corporation to aid users.

The FLOWTRAN system is installed on a CDC 6600 computer in Kansas City, headquarters of UCS. There are two ways of accessing the system: by slow-speed terminals (Remote Job Entry or RJE) or by high-speed terminals (Remote Batch Entry or RBE). In practice, most users have found a high-speed terminal is more economical. Details on the job control language procedures for accessing FLOWTRAN from either type of terminal are provided in a manual [9], also developed by the CACHE Corporation.

The early history of this FLOWTRAN project was documented in an article which appeared in this journal [10]. More recently, the CACHE Corporation completed the development of a manual [11] of demonstration exercises in process simulation using FLOWTRAN. This manual contains 27 such exercises, and has been found to be a very valuable instructional aid in providing useful and practical material for student assignments.

In its present form, roughly the first half of this computer-aided design course is devoted to

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study and usage of the FLOWTRAN system. Thus, the formal student text for this part of the course is the one developed by the CACHE Corporation [8]. In theory, usage of the FLOWTRAN system requires no knowledge of any source language such as Fortran. That is, input data to this system consists of a process description, listing of chemical components present, physical properties options, equipment and operating parameters, descriptions of feed streams and estimates of recycle streams. A main or driver program, which calls the various appropriate FLOWTRAN subroutines and functions for a particular process simulation, is then constructed automatically by the FLOWTRAN system on the basis of the input data supplied.

In order to give the students a greater knowledge and appreciation of how a system such as FLOWTRAN works and what it actually does for them, in the second half of this course process simulation studies are performed by the students using a very modest computer-aided process design system developed here at Georgia Tech. This system was developed primarily as a pedagogical tool for instructional purposes and, while similar in structure to FLOWTRAN, lacks many of the sophisticated features common in other process simulation systems. A brief description of this small process design system appeared in a recent compilation of computer programs for chemical engineers [12]. When using this system, the students must themselves construct the main driver program and set up the input/output data procedures, which are done automatically for them when using the FLOWTRAN system. A user's manual [13] has also been prepared for this system. Copies of this manual, which then serve as the second student text in this course, are distributed to the students.

A variety of example chemical processes for laboratory exercises on computer-aided design and simulation has been employed in this course over the past six years.

Maintaining continuity of course materials from one year to the next is always a problem in undergraduate engineering courses, particularly elective ones. This system is used sparingly between course offerings. It is also desirable to minimize the amount of time required to familiarize new students with the system and the coding therein. Thus, all of the subprograms (unit operation building blocks and physical property utility routines) are written in Fortran according to rather rigid programming standards. These standards have been described elsewhere [14].

TABLE II
Topics Normally Covered in the Lectures

- Structure of computer-aided design systems
- Estimation and computation of physical properties:
  - Thermodynamic
  - Transport
- Vapor-liquid and liquid-liquid equilibria
- Shortcut procedures for the design/simulation of distillation columns (Fenske-Underwood-Gilliland method)
- Shortcut procedures for the design/simulation of absorbers and strippers (Edmister method)
- Simulation of heat exchangers using the concept of heat exchanger effectiveness and number of transfer units (NTU)
- Simulation of chemical reactors
- Usage of graph-theoretic methods to identify:
  - Recycle loops in chemical processes
  - Candidates for co-sited manufacture in chemical plant complexes
- Development of design calculation precedence orders

COURSE CONTENT

A WIDE VARIETY OF topics, directly or indirectly related to computer-aided process design, is normally covered in the lecture periods of this course. Some of these lectures cover various (generally shortcut) design or simulation procedures for various chemical engineering unit operations. Repetition of material presented in earlier courses of the curriculum is generally avoided. There is also considerable discussion of methods for estimating and computing physical properties, both thermodynamic and transport, of chemical compounds. Some more specialized topics, perhaps peripheral to computer-aided process design, are also generally presented (several of these are discussed below). A summary of all of the topics normally covered in the lectures of this course is given in Table II.

Two of the specialized topics discussed in this course are given at the bottom of Table II. Several lecture periods are devoted to the development of incidence, adjacency, reachability and intersection matrices in conjunction with the identification of recycle loops in chemical processes, as described by Crowe and co-authors [7]. The usage of these graph-theoretic methods to identify potential candidates for co-sited manufacture in chemical plant complexes is also treated [15]. Another topic which is the subject of several lecture periods is the development of process design calculation precedence orders, as described by Rudd and Watson [16] in their text on the strategy of process engineering. While these supplemental topics do not represent integral parts of the computer-aided design systems used, student reaction to this relatively new material has generally been quite good.

COURSE EXPERIENCE

A VARIETY OF EXAMPLE chemical processes for laboratory exercises on computer-aided design and simulation has been employed in this course over the past six years. Some of these, and their sources, are listed in Table III. These range in

TABLE III
Process Simulation Exercises

Separation of a mixture of benzene, monochlorobenzene and hydrogen chloride [8]
Multicomponent distillation of a hydrocarbon mixture [8]
Multiple process configurations for heating and mixing of a mixture of hydrogen, methane and aromatic compounds [11]
Isothermal flash of a hydrocarbon mixture with recycle [17]
Disproportionation of toluene to benzene and xylenes [18]
Direct oxidation of ethylene to ethylene oxide [19]

complexity from relatively simple to exceedingly complex. Thus, the exercises involved with multicomponent distillation of a hydrocarbon mixture [8] and isothermal flash of a hydrocarbon mixture with recycle [17] are generally completed with relative ease by most students. On the other hand, computer simulation of the processes of disproportionation of toluene to benzene and xylenes [18] and of the direct oxidation of ethylene to ethylene oxide [19] represent extremely comprehensive and difficult exercises. Among other complexities, such as a multiplicity of recycle loops, simulation of these processes requires the construction of specialized reactor subroutines, which must be compatible with the process design system employed, and incorporation of these subroutines into the computer simulation. It has been found useful to break such complex processes down into smaller parts, and to assign only the simulation of the resulting sub-processes as student exercises.

Student response to this course has been quite good; lowerclassmen who have recently completed their introductory computer programming course often inquire about this elective course as a means of pursuing advanced studies of computer applications. A number of graduates of this course are now working in the area of computer-aided design in industry. It is extremely valuable to the instructor if the teaching assistant and one or more of the students in the course are intimately familiar with the local computer center and its operating procedures.

FUTURE PLANS

AS DISCUSSED ABOVE, this course has been offered during the spring quarter at Georgia Tech for each of the past six years. And, as a result, most of the students who elect this course do so in the final quarter of their senior year, and are thus taking this course concurrently with their required senior-level course on plant design. The original rationale for this scheduling was that a prerequisite for this computer aided design course should be chemical reactor design, which is normally taken in the winter or second quarter of a student's senior year. This scheduling has basically been found to be a workable arrangement. In recent years, however, a large number of students have expressed the wish that this elective course be offered in the winter quarter, before they enter the plant design course. In this manner, they would have their entire training with FLOWTRAN behind them before plant design. With the present arrangement, the students are about halfway through their plant design course before they are reasonably facile with FLOWTRAN, and as a result the latter tool is of little or no use to them in plant design. Also, the course experience has been that, because of the complexities involved and other topics covered, there is scant opportunity to effectively work in computer simulation of chemical reactors in this elective course (see above discussion). Accordingly, beginning

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with this academic year, this elective course is to be offered during the winter quarter, and the primary prerequisite course will be chemical engineering thermodynamics. Again, course experience has been that thermodynamics, which in timely fashion is normally taken by the students in the first or fall quarter of their senior year, is indeed perhaps the most important prerequisite, at least insofar as it forms the basis for physical property estimation and vapor-liquid equilibria calculation procedures. By this time, most students would also have completed their unit operations sequence of courses (which would also be obviously essential). There is no great loss with respect to reactor design, since most students would be taking the reactor design and computer-aided process design courses concurrently.

One can look forward to future interesting and exciting developments in the general area of computers in chemical engineering education. The CACHE Corporation has recently published a prospectus [20] to explore the possibility of creating a library of large-scale computer programs for use in chemical engineering education and research. Some of the programs currently being considered include: evaluation of alternate energy recovery systems, computer-aided control system design, computer package for the design and rating of multi-product batch plants, computer program for synthesis of flow sheets for continuous chemical processes, programs for computing vapor-liquid equilibria, and a physical property data service. The hope is that these programs could be installed on a computer network, similar to the mode of access to FLOWTRAN, and made available at reasonable cost to academic users. The ready availability of such programs would impact favorably not only upon an elective computer-aided process design course such as described herein, but also upon many of the other courses in the required chemical engineering curricula at most schools. □

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ChE conferences

ADVANCED SEMINAR ON DYNAMICS AND MODELLING OF REACTIVE SYSTEMS

• The Mathematics Research Center at the University of Wisconsin-Madison will hold at Advanced Seminar on Dynamics and Modelling of Reactive Systems, October 22-24, 1979. Lecturers will include N. R. Amundson, R. Aris, D. G. Aronson, G. F. Carrier, M. Feinberg, E. D. Gilles, P. S. Gough, L. N. Howard, J. B. Keller, D. Luss, J. Rinzel, R. A. Schmitz, J. H. Seinfeld and F. A. Williams. A detailed program will be available in August. Further information may be obtained from Mrs. Gladys Moran, Mathematics Research Center, Univ. of Wisconsin, 610 Walnut Street, Madison, Wisconsin 53706.