CHEMICAL PROCESS DESIGN AND ENGINEERING*

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The aim of this workshop was to present novel teaching techniques and instructional formats, as well as to present results of recent research which lend themselves toward course material for design and process engineering. Both undergraduate and graduate design instruction were considered.

BERKELEY GRADUATE PROGRAM

The graduate program in Process Design and Engineering at Berkeley was described by Grens. This undertaking started informally with the introduction of courses and theses by several faculty members and grew into a coherent program which received grant support from the NSF Advanced Science Education Program in 1968.

The program has no prescribed curriculum but offers some design exposure for many graduate students with more concentrated work, and design-oriented theses, for those with a primary process engineering interest. Students have been enthusiastic about the courses, and the desire for both M.S. and Ph.D. theses in this area has exceeded the available financial support.

In the six identifiably design-related graduate courses teaching methods include lectures and ordinary problem work, but great emphasis is also placed on the use of short case problems.[1] Computer implementation is included where appropriate. Several persons from industry have presented courses and seminars. About 20 theses have been completed in the program to date. These remain subject to the requirement for an original contribution, and the results are often published[2,3,4].

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PROCESS ANALYSIS

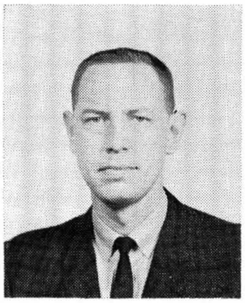
King discussed a class problem in which the students are presented with a flow diagram and operating conditions for an ethylene plant. About 20 discussion questions are brought up, relating to the function of each item of equipment, the reasons for the particular ordering of equipment, reasons for the particular operating conditions, and possible alternative process configurations. Homework includes performing supporting calculations to define in what ways thermodynamics and kinetics of various reactions govern the reactor conditions, to select appropriate operating pressures for distillation columns, etc. A similar problem involving hydrodealkylation of toluene to benzene is available[5].

Several examples of trouble-shooting problems were discussed by Lynn. In this type of problem the student is presented with a description of a malfunctioning piece of equipment or simple process, and must deductively devise a series of questions and proposed tests which implement an efficient strategy for diagnosing the cause of the malfunction. This approach has been described by Woods and Silveston[6]

PROCESS SYNTHESIS

Rudd concentrated on the general principles of process synthesis.[7] His detailed discussions of the workshop were expanded in a general lecture examining the teaching of process synthesis as the first course in engineering.

Process flowsheet synthesis deals with bringing together the diverse concepts of engineering to form a coherent whole which is the process flowsheet describing the proposed process system. Prior to 1968 little attention had been given to the development of general principles of synthesis.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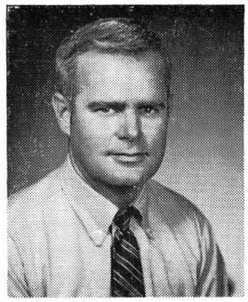
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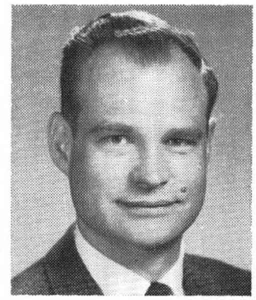
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However, in recent years work has accelerated and significant progress has been made.[8]

In particular, Rudd discussed the branch and bound methods of synthesis with reference to the synthesis of networks of heat exchangers, heaters and coolers.[9] By forming boundary problems which are more easily solved, the flowsheet can be synthesized which recovers heat energy most economically. The second topic was the use of list processing methods in combination with dynamic programming for the synthesis of separation systems.[10] The final topic discussed in the workshop sessions was the synthesis of the whole process using the decomposition and heuristic methods of Siirola and Powers.[11,12]

King presented a relatively structured case problem involving the design of demethanizer columns for ethylene plants.[13] This problem and another in which methane liquefaction processes are generated using the digital computer stem from thesis research on "evolutionary" approaches for process synthesis.[14] In the demethanizer problem the class generates a process and is then given the results of equipment sizing and cost analysis. A hopefully better process is evolved by endeavoring to reduce the most important cost components of the current process, and the entire procedure is repeated a number of times.

Lynn discussed two more qualitative problems involving process synthesis. The first was a short introductory example of the open-ended design problem, in which the student is asked to extract the most possible refrigeration from a high-pressure gas stream passing through to a low-pressure pipe line. The student must decide upon a suitable criterion for "most possible" as well as choosing various methods for extracting refrigeration from the stream. The second problem was an example in which students faced with the need for desalting a sulfate-rich brackish water consider the possibility of using well-established Solvay technology in their solution.[15] The student is asked to supply the missing link in the processing cycle on the basis of hints given in the problem statement.

PROCESS SIMULATION

Grens outlined a graduate course dealing with simulation of continuous chemical processes at the steady state by mathematical models implemented with computer programs. Concurrent reading is from the recent and current literature —e.g., Christensen and Rudd,[16] Westerberg and Edie,[17] Upadhye and Grens.[18]

The course begins with discussion of the nature of simulation, computational background, and process description and specification. Then the primary subjects are considered: calculation of recycle systems and simulation of individual process units. Finally, the development of integrated process simulations and use of general purpose process simulation programs are discussed.

Two evolutionary case problems are utilized. One is of large scope but is not treated in detail; it is used to allow examination of decomposition methods and has sufficiently complex loop structure to be useful for this purpose. The other problem is of quite limited scope in order to permit detailed computer simulation by each student. It is designed to illustrate unit simulations and alternative convergence procedures.[19]

PROCESS OPTIMIZATION

Foss described a graduate course in which the proven methods of optimization are applied to problems of process design and operation. Emphasis is placed on approaches to problem formulation and solution.

Constrained problems are discussed first because nearly all realistic process optimization problems involve minimization under constraints.

Linear programming is treated first because of its conceptual simplicity and because students are equipped in a week's time to try their skill at formulation of a complicated refiners scheduling problem (about 35 constraints). The constrained nonlinear problem is introduced by an example (see below) in which the tasks of stating the objective function, selection of variables, identification of constraints, and choice of a minimization method are shown to be highly interdependent. Definitions and conditions for constrained minima are discussed followed by gradient projection methods and penalty function methods.

Unconstrained minimization methods such as pattern methods, conjugate directions without derivatives, the gradient methed, the Davidon-Fletcher-Powell method, and quasi-Newton methods are discussed along with one-dimensional search methods needed for most of these techniques. Dynamic programming is briefly discussed and is shown to be of some, but limited, usefulness in process optimization calculations.

Concurrently, students are engaged in developing a solution to a heat exchange case problem. This is a nonlinear, constrained problem involving the optimal design of a simple (4 variable) heat exchange network, and is assigned to students in a series of 3 or 4 homework assignments. Solution of the problem involves formulation of the objective function, constraints, process modeling, selection and programming of a constrained minimization method. The problem admits alternative sets of design variables, the choice of which determines the linearity or nonlinearity of the constraints. Both gradient projection methods and penalty function methods may therefore be used. Discontinuities in the objective function arising from a maximum size condition on the exchangers complicate the one-dimensional searches needed in these approaches. Various considerations needed for the solution are treated in a series of lectures coordinated with the students' progress on the problem. One complete calculation requires about 10 seconds (CDC 6400), but students are found to spend about 13 minutes of computer time each in the development of their programs. □

Editor's Note: Titles of the case problems referred to in reference [1] *and available from Professor C. J. King are: Production of benzene and xylene by hydrodealkylation. Simulation of a hydrodealkylation plant. Continuous drying of air. Removal of water vapor in freeze-drying. Desalination by reverse osmosis. Sulfate removal from brackish water. An evolutionary problem in process simulation. Removal of inerts from ammonia synthesis gas.*

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