THE USE OF FLOWSHEET SIMULATION PROGRAMS IN TEACHING CHEMICAL ENGINEERING DESIGN

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The chemical engineering design student is required to calculate the material and energy balance, the size and cost of equipment, the operating cost, and some profitability criterion for each process he studies. Once the student has mastered these procedures by hand computation, repetitive calculations become monotonous and time consuming. The result is that often little time is available for the study of design principles.

A computer flowsheet simulation program, named CHESSE, has been developed at the University of Missouri-Rolla that does the above calculations and provides the user with the profitability of the simulated process. The development of the CHESSE program is discussed and several examples of processes simulated by design students are presented.

The use of CHESSE during the latter part of the design course has been found to enhance the student's education in this area. Additional cases can be studied in synthesizing and analyzing the optimal process and a better grasp by the student of design principles is apparent.

THE PROCESS OF EDUCATING chemical engineers culminates in the design course. This course requires the student to apply the basic technology from other courses, such as thermodynamics and transport operations, to predict the performance and economics of chemical systems.

Students often realize, for the first time in the senior design course, the practical application of much of the course content of their undergraduate curriculum. It is, therefore, essential that the design course be a comprehensive integration of technological principles from earlier courses with design and economic procedures.

Comprehensive design coverage represents a challenge to educators who must often accomplish this coverage in three semester hours. Consequently, new and innovative methods are constantly being sought to improve the teaching efficiency.

One innovative teaching technique is the use of flowsheet simulation programs for the solution to classroom design problems.

FLOWSHEET SIMULATION PROGRAMS

ONE SUCH INNOVATIVE teaching technique is the use of flowsheet simulation programs [1,2] for the solution to classroom design problems. These programs define the chemical process material and energy balances from a description of the equipment in the process [3].

A typical design problem is the ethylene process [4] shown in Figure 1. Ethylene is produced by cracking ethane and propane. The product is purified in three distillation columns. Hydrogen and methane are recovered for fuel, and ethane is recycled. Propylene and heavier hydrocarbons are by-products.

The material and energy balance data for the ethylene process are shown in part in Figure 1. These data could be obtained by hand calculation or a flowsheet simulator could be employed to provide this information.

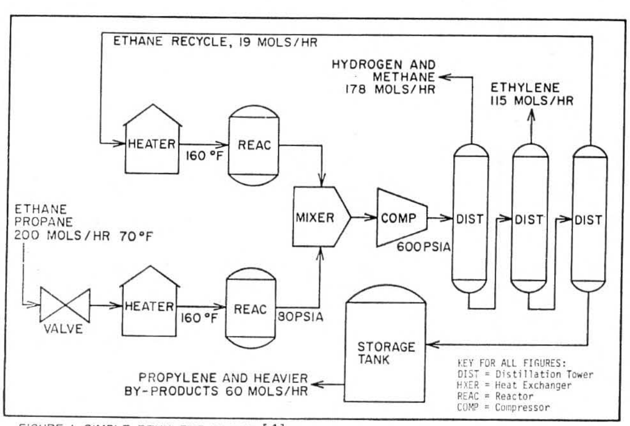


FIGURE 1. SIMPLE ETHYLENE PLANT [4]

The design student must proceed, exactly as would the computer, in calculating material and energy balance relationships for such a process. Once the basic concepts are understood by the student, these calculations become routine and time consuming. Thus, the use of a simulation system removes some of the monotony from the design course and allows more emphasis to be placed upon the principles of design. The incorporation of flowsheet simulation programs in teaching design has been practiced for many years at several universities [5].

Design, of course, does not stop with the material and energy balance, but culminates with economic analysis of the process which leads to an optimal design [2]. In making an economic analysis, the student is required to make detailed estimates of the equipment and operating costs in the process. The procedure of cost estimating must be repeated for each case studied in arriving at the optimal design. Again, such procedures are routine, time consuming, and afford little learning value to the student.

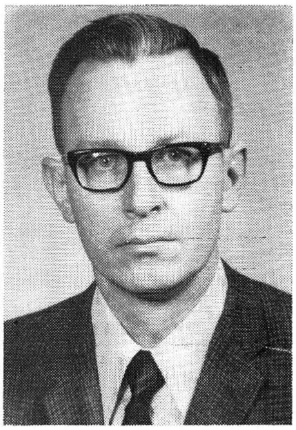
The University of Missouri has developed a simulation program, named CHESSE (*C*hemical *E*ngineering *S*imulation *S*ystem with *E*conomics), [6] which does the cost estimating and provides a complete economic analysis of the chemical process. This program is a modification of the basic CHESS system [4]. The purpose for developing such a program was to enhance the teaching of design. Several advantages were expected:

- **Provide the student the opportunity to study more processes.**
- **Provide the student the means of arriving at a better design since more cases can be studied in searching for the optimum.**
- **Introduce the student to computer oriented design methods used by industry.**

The purpose of this paper is to discuss the development of the CHESSE program and to report on its use in teaching design. A basic understanding of flowsheet simulation programs by the reader is presumed.

CHESSE

Economic analysis is the determination of some economic criterion, such as return on investment, that can be used to judge the worth of the system under study. The choice of the best process *design* is made by reviewing the economic criterion for all processes studied and choosing the process that maximizes the profitability. The basic information required for calculation of an economic criterion is the investment and profit.



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The economic calculations can be done on the computer and are easily integrated with the usual flowsheet simulation programs which provide much of the data for the economic balance. The computations can best be done in a stagewise manner. First, the material and energy balance must be converged for all recycle loops. Then the plant investment, which is dependent upon the material and energy balance, can be determined. Finally, the profit, which depends upon the investment as well as the material and energy balance data, is found. The procedures used in CHESSE to find the investment and profit will be summarized.

DETERMINATION OF INVESTMENT

The total investment for a chemical process is made up of the cost of the process equipment plus the cost of auxiliary facilities, such as the supply of utilities. The auxiliaries cost can generally be calculated as a function of the investment in process equipment. Therefore, the total investment can be found from the size and cost of each individual item of equipment within the process.

The basis for sizing and costing the equipment in the CHESSE program is given in Table 1. Most of the data for these computations is available from the material and energy balances and only a minimum amount of additional information must be supplied by the student.

The cost calculations for each equipment item

TABLE 1. SUMMARY OF DATA FOR DETERMINATION OF EQUIPMENT SIZE AND COST IN CHESSE

Equipment	Cost Basis	Design Basis in CHESSE	Data Source
Distillation Tower	Tower height, diameter, material of construction, and type of trays	Number of trays by Fenske, Underwood, Gilliland procedure [7]. Tray by tray determination also available. Tray spacing set at 2 ft. Tower diameter by maximum vapor velocity method of Souders and Brown [8]	Reflux ratio, type of tray and material of construction by programmer. Flow rate and thermodynamic properties from CHESSE.
Absorber	Height, diameter, material of construction, and type of tray or packing	For packed columns, height based on absorption factor method [9], and diameter based on flooding velocity method of Lobo [10]. For tray towers diameter found as in distillation.	Programmer specifies type of column, material of construction. Other calculations by CHESSE.
Flash Column	Height, diameter, and material of construction	Three feet of liquid holdup provided. Three feet of vapor disengaging space provided. Diameter same as for distillation.	Flow rates and thermodynamic properties by CHESSE. Material of construction by programmer.
Heat Exchanger	Area, material of construction, number of passes and shells, and type exchanger	Area from heat duty, overall heat transfer coefficient and logarithmic temperature difference.	Heat duty and temperatures from energy balance. Coefficient and other data by programmer.
Reactor	Volume, material of construction, and type of reactor	None	Programmer must specify volume, material of construction and type of reactor.
Pump and Compressor	Capacity, type of pump and drive, pressure rise and material of construction	Work of compression calculated from specific heat ratio. Pump work from product of flow rate and pressure rise [4].	Programmer specifies pressure rise, type of material, and whether spare pump is needed.
Valve	Diameter and material of construction	Valve Diameter as pipe diameter to give liquid velocity of 4 fps or vapor velocity of 10 fps.	Material of construction specified by programmer
Tank	Volume and material of construction.	Tank Volume from flow rate and desired holdup.	Flow rate from material balance. Holdup and material of construction by programmer.

are based on the modular cost concept of Gutherie [11]. The cost computed is the total installed cost including foundations, piping, wiring, instrumentation, etc. For each piece of equipment, the cost depends upon the equipment size, material of construction, pressure, and specific type, such as steam or gas fired heat exchanger. The size is computed by CHESSE from the appropriate flow rate and design equation. Pressures are available from the energy balance. The programmer must specify equipment type and material. Options are available for the programmer to specify the cost separately for any piece of equipment, if the methods for costing in CHESSE are not appropriate. All costs in CHESSE are from 1970 data and provision is made to adjust these costs to the present time by use of the Marshall and Stevens Index [13].

The total process equipment cost is found by adding the costs for the individual items of equipment in the process. Auxiliary equipment costs are then found according to the percentages given in Table 2 [12]. These percentages total about 40 percent of the process equipment cost, and the programmer may change this percentage, if desirable. CHESSE assumes a Gulf Coast location and a location factor is provided for adjusting the cost for a difference in geographic location. Contingency is then added to give the total investment. A contingency of 10 percent is added by the program, but the programmer has the option of varying this percentage.

REVENUE, OPERATING COST, AND PROFIT

The basic data for the determination of revenue and process operating cost in CHESSE is summarized in Table 3. These data are computed from the total investment and material and energy balance information.

The method of computation and the source of the data are also given in Table 3. Revenue and raw materials cost are calculated from the product and input stream flow rates supplied by the material balance. Stream prices are furnished by the programmer. Utilities costs are determined from the energy requirements and the prices for power, fuel, steam and water. Labor requirements are found from the Wessel correlation [14]. Other fixed costs are determined as a percentage of the

Table 2. Summary of Investment in Auxiliary Facilities for Chemical Process Plants

Auxiliary Facilities	Percentage of Installed* Process Equipment Cost Added [12]
Process Piping	20.0
Yard Improvement	
Land Cost	2.0
Site Clearing	0.6
Parking Areas	0.2
Landscaping	0.1
Yard and Fence Lighting	0.2
Other Improvements	0.4
Utilities	
Steam Generation	3.0
Steam Distribution	1.0
Water-Supply, Cool and Pump	1.8
Water-Distribution	0.9
Water Treatment	0.6
Electric-Main Substation	1.5
Electric-Distribution	1.0
Gas Supply and Distribution	0.3
Air Comp. and Distribution	1.0
Sanitary-Waste Disposal	0.3
Service Facilities	
Auxiliary Buildings	5.0
Railroads	0.6
Fire Protection System	0.7
Communications	0.2
Location Factor	
(Basis—Gulf Coast Location)	0.0
Contingency	10.0

*NOTE: Installed equipment cost includes equipment instrumentation, wiring, piping, minor steelwork, concrete foundations, substructures insulation, and painting.

total investment, labor cost or working capital. Cost items such as advertising, product distribution and research are computed as a percentage of revenue [12]. CHESSE uses industry wide average utilities prices or percentages to compute these costs. The programmer has the option of specifying values different from these averages, if desirable.

The total operating cost is the sum of the items, except revenue and working capital, given in Table 3. The before-tax earnings are computed as the difference between the revenue and total operating cost. Income taxes are figured as a percentage of the before-tax earnings and are subtracted from before-tax earnings to give net profit.

The cash accumulation is calculated as the sum of net profit and depreciation. CHESSE presently computes two economic criteria; return on investment and payout period. The return on inventment is the net earnings divided by the investment expressed as an annual percentage. The payout period is the investment divided by the cash accumulation.

If desired by the programmer, the investment and economic calculations in CHESSE can be bypassed entirely.

TEACHING EXPERIENCE WITH CHESSE

The experience with the use of CHESSE in the classroom has been encouraging. Several examples of the types of problems the students have solved will exemplify the kinds of results obtainable from a program such as CHESSE.

Ethylene Process

The ethylene process shown in Figure 1 was simulated by the design students using CHESSE. This plant was designed to produce 115 mols/hr of ethylene for 330 days per year, i.e., 25 million pounds per year. A total investment of $1,008,965 is required. The investment summary of individual equipment items is also available from CHESSE.

A total operating cost of $1,445,715 is computed. This represents a cost of ethylene of about 3.5 cents per pound, allowing credit for by-products. By comparison, Gutherie [15] gives the investment for this size ethylene plant as $1,100,000 and the operating cost as 3.2 cents per pound.

With an ethylene price of 4 cents per pound, the return on investment is 6.2 percent per year and the payout period is about 7 years. From this initial design, the students proceed to evaluate the effects of larger plant sizes, product price and process variables on the economics of the ethylene process.

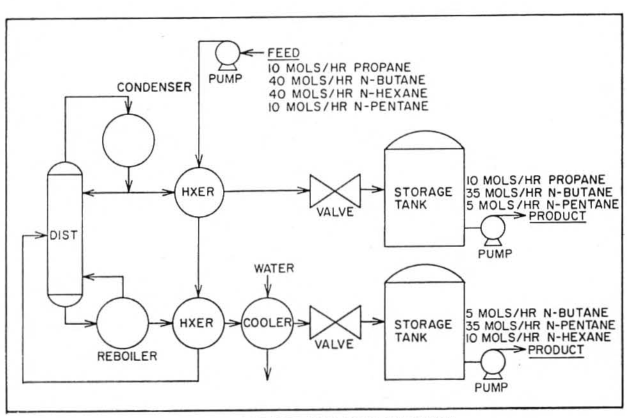

FIGURE 2. SIMPLE DISTILLATION PROCESS WITH HEAT RECOVERY

Simulation of this process requires about 20 seconds of computer time on an IBM-360-50 machine.

Hydrocarbon Distillation Optimization

A simple distillation column with heat recovery, shown in Figure 2, is used to illustrate optimization principles. The column splits a multicomponent paraffin mixture and the products exchange heat with the feed. The process variables for optimization are tower pressure, column reflux ratio and approach temperatures in the heat exchangers.

Benzene Process

Figure 3 is a typical process for the hydrogenation of toluene to produce benzene. Hydrogen and toluene are heated to 1250°F and reacted at

TABLE 3. SUMMARY OF ECONOMIC DATA FOR DETERMINATION OF OPERATING COST IN CHESSE

Data	Method of Computation	Source of Data	Options
Working Capital	(5 percent of Investment) + (8 percent of revenue)[12]	Investment and revenue calculated by CHESSE	Other percentages may be specified by programmer.
Revenue	Σ[(Volume of product streams) x (product prices)]	Volume of product streams from material balance. Prices furnished by programmer.	
Utilities Cost			
Electricity	(Power consumed) x ($.01/kwh)	Power consumption from energy balance.	Alternate unit power, fuel steam and water costs may be specified by programmer or programmer may specify utilities cost in any equipment item.
Fuel	(Fuel consumed) x ($.30/mm BTU)	Fuel consumption from energy balance.	
Steam	(Steam consumed) x ($.65/mm BTU)	Steam consumption from energy balance.	
Water	(Water consumed) x ($.10/m gal)	Water consumption from energy balance.	
Raw Materials Cost	Σ[(Volume of Incoming Streams) x Prices)]	Quantity of incoming streams from material balance. Prices specified by programmer.	
Operating Supplies	(6 percent of labor) + (catalyst cost)[12]	Labor cost from CHESSE. Catalyst cost by programmer.	Percentage may be varied by programmer.
Labor Costs	(Operating labor hours/yr) x (labor cost/hr)	Man hrs = [tons product](10)(N)/(Capacity, tons/day)$^{.75}$[14] where N = number of process steps. Capacity, production and number of steps found by CHESSE. Labor cost/hr of $3.50 is used.	Alternate hours or cost may be supplied by programmer.
Supervision	20 percent of labor cost [12]	Labor cost from CHESSE	Percentage Variable
Payroll Burden	(.25) x (labor cost + supervision) [12]	Labor cost and supervision from CHESSE	Percentage Variable
Overhead	(.5) x (labor cost + supervision) [12]	Labor cost and supervision from CHESSE	Percentage Variable
Maintenance	5 percent of investment [12]	Investment from CHESSE	Percentage Variable
Taxes and Insurance	2.5 percent of investment [12]	Investment from CHESSE	Percentage Variable
Depreciation	(1 - Salvage Value) x (Investment) ÷ Depreciable life	Investment from CHESSE. Salvage value = 10 % of investment	Salvage value and depreciable life are variable
Interest	(.1) x (Investment + Working Capital)	Investment and working capital from CHESSE	Percentage Variable
Sales and Advertising	15 percent of Revenue [12]	Revenue from CHESSE	Percentage may be varied by programmer
Administration	6 percent of Revenue [12]	Revenue from CHESSE	Percentage Variable
Product Distribution	3 percent of Revenue [12]	Revenue from CHESSE	Percentage Variable
Research and Development	10 percent of Revenue [12]	Revenue from CHESSE	Percentage Variable

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800 psia. The effluent from the reactor is separated by a series of flash and distillation towers. Hydrogen and toluene are recycled bback to the reactor.

CONCLUSIONS

At the University of Missouri-Rolla the CHESSE program is not introduced into classroom use until about the middle of the design course. At this time, the student has been through several equipment design problems and at least one detailed process design by hand calculation. The procedures of making material and energy balances, sizing equipment, cost estimation, economic analysis, and optimization have been mastered. The use of CHESSE is not to teach these procedures, but rather to facilitate their use in learning design principles.

The use of CHESSE requires no special or prior computer programming skill. The NAMELIST format is used to furnish all data for the program. These procedures are quite simple and the student usually is ready to design a process on the computer with a few hours instruction and practice.

During the second half of the design course, after CHESSE has been introduced, the student will design and optimize about three complete chemical processes, such as those shown in the earlier examples. The optimization may involve several variables and advanced optimization techniques are introduced. The class may work on the same process at one time, but each student can be assigned a different problem by changing the plant size or some other parameter of the system.

Students seem to enjoy the use of CHESSE. More importantly, they seem to obtain a deeper grasp of design principles. The economic effect of changing values of a variable become readily apparent. Important variables are more readily distinguished. The point of diminishing returns in optimization becomes real. Computer design permits study of areas, such as plant location and distribution costs, that do not receive much attention otherwise. Furthermore, the area of process synthesis can be stressed since the student has more capability in the allotted time for modifying processes.

It is not implied that the CHESSE program provides the ultimate in design education. Many refinements and improvements are still needed. Improved thermodynamic capabilities, additional unit operations, more precise methods of equipment sizing, and better cost estimation are some of the areas that are under study.

The student should never use a computer unless he knows exactly what the machine is doing. Therefore, he should always be required to do process design calculations by hand. However, the subsequent use of computer aided design programs can be used to enhance his education. □

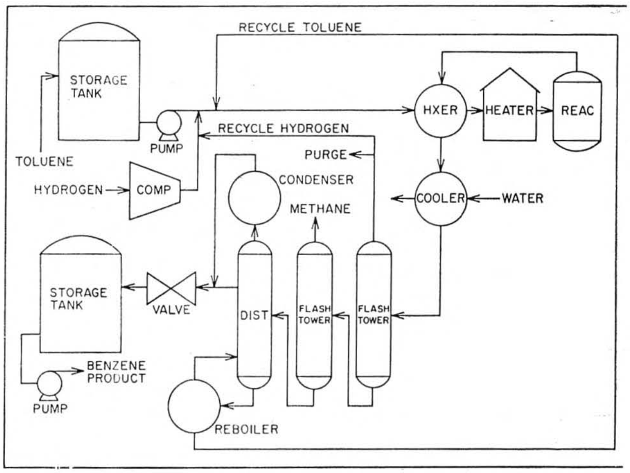

FIGURE 3. BENZENE PROCESS

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