SIMULATION OF THE MANUFACTURE OF A CHEMICAL PRODUCT IN A COMPETITIVE ENVIRONMENT

T. W. F. RUSSELL, D. F. BRESTOVANSKY
and R. L. McCULLOUGH
with the assistance of C. K. WANG
University of Delaware
Newark, DE 19711

A MAJOR CHALLENGE FACING engineering educators is the infusion of notions of competition, uncertainty, and risk-taking into the deterministic methods traditionally used in the instruction of engineering students. An educational tool was described in a previous article [1] which utilized computer simulation techniques to provide an evaluation of a process design in a more realistic fashion than the usual procedure of "grading" a design report. In this article, we describe an advanced simulation which illustrates how basic engineering skills can be combined with economic considerations and risk-taking judgments in order to effectively design and operate a chemical processing unit in a competitive environment.

For this advanced simulation, data are provided to establish a design concept, capital cost, and operating cost. The completion of the design requires the specification of the production capacity (or "size") of the plant. This crucial decision is left to the participants and is based on their judgments concerning the uncertainty of market projections as well as their appraisal of the behavior of the competition. This decision is further confounded by the the availability of other options which compete for the limited funds available ($9 million). Research and development programs are proposed which may have potentially high returns. However, the commitment of funds to these high risk projects reduces the funds available to build the processing plant and leaves open the possibility of not being competitive in an established market place. Information concerning the estimated risks involved in the research and development programs is provided so that rational qualitative judgments can be made concerning the disposition of limited funds. These elements of risk associated with the pay-off from the research and development projects along with possible fluctuations in the market and the uncertainty associated with the actions of competitors are intended to illustrate the difficult conditions under which many important engineering decisions are made.

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This simulation has been used as one of five projects in Technical Project Management, a course of the Chemical Engineering Department of the University of Delaware. This course is open to advanced seniors, graduate students, and practicing engineers. Their enthusiastic response to the simulation project has provided the motivation for this article.

DESCRIPTION

The participants are grouped into four competing teams with 4 to 5 members per team. Each team is provided with technical, marketing, and economic information in the form of memoranda in order to familiarize the participants with this important form of communication. The central theme of the project is the design and operation of a plant for the manufacture of a primary product "D". A by-product "C" is produced that can be a potential source of profit. Each group is allotted an initial sum of $9 million to finance the project.

The first simple task involves the determination of the rate constant from concentration-time data for the catalytic decomposition of raw material "A" into the product "D" and by-product "C" via the reaction:

$$A \rightarrow \frac{1}{2} C + D$$

A simple process with an isothermal continuous flow stirred tank reactor and distillation column can be used to manufacture "D" and "C". The process flow diagram is shown in Fig. 1 and described elsewhere [2]. Relationships that can be used to estimate the capital cost, operating cost, and materials cost are given in the memoranda. The information contained in these various memoranda can be easily formulated into an economic model for the process unit cost as a function of plant capacity by procedures described in engineering textbooks [3].

Estimates for the total demand and associated selling price for the primary product "D" are provided for a ten year period with the caution that these estimates may be in error by approximately 15%. The price-quantity data given are thus in the form of a standard demand curve used by the microeconomist. The marketing data for "D" provide a basis for judgments concerning the specification of plant capacity (reactor size, distillation column capacity). This crucial decision requires judgments concerning (i) the market share that can be obtained in relationship to the possible strategies and behavior of competing teams, and (ii) the uncertainty of the market projections.

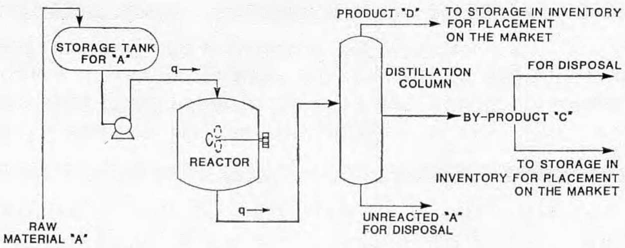
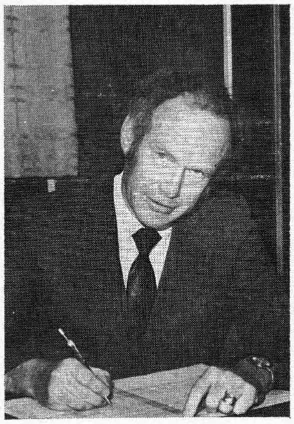
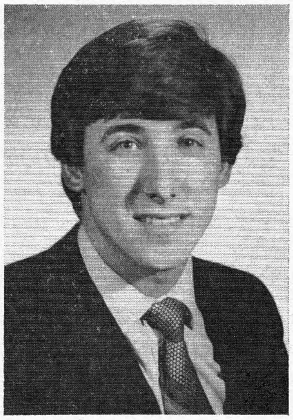
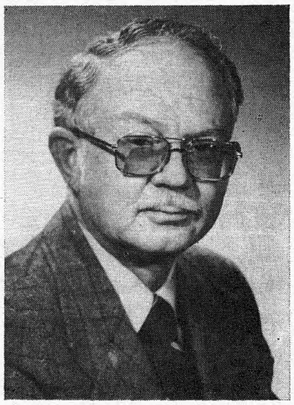


FIGURE 1. Process flow diagram

The processing unit size and capital cost decision is made more difficult by the availability of options, all of which require funds which could be used for plant construction. As one option, data concerning improvements in process efficiency and the related cost are given which can be used as a basis for a "cost-benefit" analysis. These data are constructed to illustrate the option for an optimum investment in process related research. In a second option, a research and development program is proposed which could lead to the potential com-







T. W. Fraser Russell is the Allan P. Colburn Professor of Chemical Engineering and the Director of the Institute of Energy Conversion, a laboratory devoted to photovoltaic cell research at the University of Delaware. He received his MSc and MSc degrees in chemical engineering from the University of Alberta and his PhD in chemical engineering from the University of Delaware. His industrial experience includes work as a design engineer with Union Carbide Canada where he designed the first multipurpose continuous chemical processing plant built in Canada, and as a research engineer for the Research Council of Alberta, where he did some initial development work on the Athabasca tar sands. **(L)**

Dennis F. Brestovansky is an Instructor of Chemical Engineering and Research Associate in the Institute of Energy Conversion's Photovoltaic Unit Operations Laboratory at the University of Delaware. He received his BS and MS degrees from the University of Delaware. Mr. Brestovansky's industrial experience includes employment as a research and development engineer with the Buckeye Cellulose Corporation in Memphis, Tenn. At the Institute, he is involved with research into the development and design of a continuous process for the manufacture of low cost, thin-film solar cells. **(C)**

R. L. McCullough, Professor of Chemical Engineering and Associate Director of the Center for Composite Materials at the University of Delaware, received his undergraduate chemistry training at Baylor University, and was awarded a Ph.D. in Chemistry by the University of New Mexico, while employed by the Los Alamos Scientific Laboratories. Prior to his appointment at the University of Delaware in 1971, he was associated with the Boeing Company as a Senior Research Scientist and Acting Director of Materials Science Laboratory; and the Chemstrand Research Center, Monsanto Company, as Group Leader and Acting Manager of the Fiber Science Section. Dr. McCullough has published technical papers and organized symposia in the areas of polymer structure, molecular mechanics, structure-property relations, and composite materials and is the author of several books. **(R)**

Upon specification of the production capacity (i.e. the anticipated share of the markets), some simple calculus can be used to obtain an optimal conversion of reactant. The distillation column is constrained by a maximum design flow rate since a flow in excess of the design limit will result in entrainment and loss of proper product specifications.

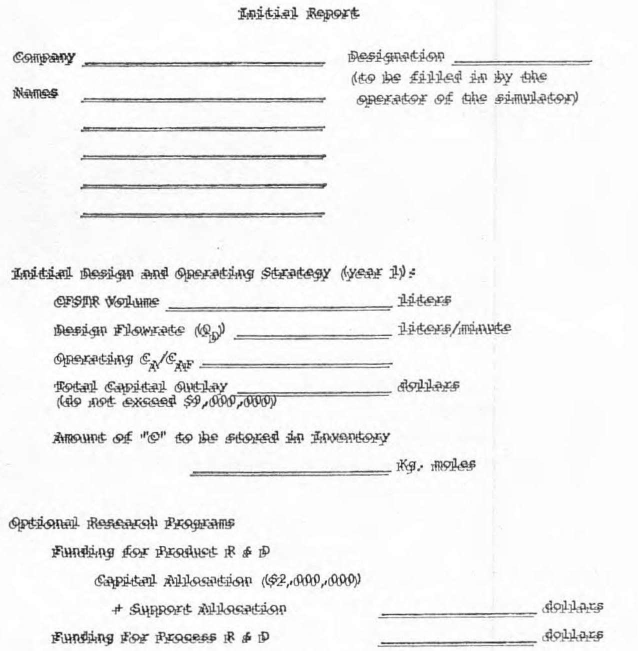
mercialization of by-product "C" and attendant new sources of income. This R&D program is a "high-risk" venture with no guarantee of success and requires an initial commitment of $2 million for pilot plant capital and then additional support each year for a research staff. The allocation of the support funds is described in terms of "normal", "crash", and "minimal" programs. "Case studies" are given to illustrate the probabilities of success under these various levels of funding. For example, under the "crash" program it is projected that a 50% chance exists for marketing "C" in Year 2 and there is a 95% chance that "C" can be sold in Year 3. For a "normal" schedule, there is a 50% chance that "C" can be sold in Year 4 and a 95% chance that "C" will be on the market by Year 6. Other case studies are given to illustrate the effects of erratic funding patterns. Again, demand and price projections for "C" are given with the caution that these projections could be in error by approximately 20%. The diversion of funds to these alternate projects reduces the capital available to build the plant and therefore reduces the capacity for producing product "D".

The development of a strategy is further complicated by a provision which allows for an expansion of production facilities in the fifth year of the simulation. In order to accomplish this expansion, the team must have generated sufficient funds from the sale of "D" (and possibly "C") in the prior years to cover the capital cost of the expansion. A team with a large R&D effort (and a small capacity plant) could accumulate sufficient funds from the early sale of "C" for a large scale expansion in Year 5. This could allow them to dominate the future market for both "C" and "D". Alternately, a team which foregoes research could build a production facility capable of generating sufficient funds, solely from the sale of "D", to finance an expansion that could maintain their domination of the "D" market.

Upon specification of the production capacity (i.e. the anticipated share of the markets), some simple calculus can be used to obtain an optimal conversion of reactant. The distillation column is constrained by a maximum design flow rate since a flow in excess of the design limit will result in entrainment and loss of proper product specifications. The teams may elect to "oversize" the distillation column (relative to the size dictated by the optimum conversion) to gain flexibility in developing a production strategy.

Each team submits proprietary reports for the initial design specifications, operating conditions, and research strategies (Fig. 2). The data for all teams are submitted to the simulator. Internal checks are conducted to identify trivial errors such as those resulting from unit conversions, etc. If design errors have been made, the value leading to a lower production rate is selected. Errors in operating conditions are adjusted to meet the design constraints, such as the flow limit on the distillation column. If the capital or research funds are allotted in excess of the current cash balance, the funds will be reduced to give a current cash balance of zero. Funds for plant construction are given priority over research funds.

In each period a random number generator is used to establish deviations away from the projected demand. The sampling procedures are de-



Initial Report

Company ____________ Designation ____________
(to be filled in by the operator of the simulator)

Names ____________
____
____
____
____

Initial Design and Operating Strategy (year 1):

CFSTR Volume ____________ liters

Design Flowrate (Q_D) ____________ liters/minute

Operating C_A/C_{AF} ____________

Total Capital Outlay ____________ dollars
(do not exceed $9,000,000)

Amount of "C" to be stored in Inventory
____________ Kg. moles

Optional Research Programs

Funding for Product R & D

Capital Allocation ($2,000,000)

+ Support Allocation ____________ dollars

Funding For Process R & D ____________ dollars

FIGURE 2. Input to simulator: Initial team report

signed so that random fluctuations of ± 15% (or less) and ± 20% (or less) may occur from the yearly market projections for "D" and "C" respectively. The selling price is established from the actual values of the market sizes through the "demand-curve" relationships. These fluctuations can have a significant effect on the teams' cash flows. The assignment of market share is biased in favor of the teams with large capacity and large inventories. The specific relationship used to establish this bias is not made available to the participants.

Progress toward the R&D breakthrough is determined by a Monte Carlo procedure which operates by sampling at random, but with the frequency of a "research probability function". The "spread" of the research probability function is established by the funding levels and patterns as reflected by a "Case Studies Summary". Although each team can influence the "odds" for a breakthrough by modifying research strategies, the breakthrough time remains an unpredictable (stochastic) event within the limits described in the "Case Studies Summary".

The inventory of the primary product, "D", is controlled by the simulator. Any unsold "D" will be stored automatically and placed on the market (along with past inventories and current production) in the following year. No provisions are available for dumping "D" so that large inventories and high inventory cost can accumulate. Deposition of the secondary product, "C", is controlled by the team, and "C" can be dumped or retained in inventory. The product "C" can only be sold from inventory. If a new product research "breakthrough" occurs and no "C" is in inventory, no revenue will be generated from the sale of "C". The amount of "C" to be placed on the market in a given year must be specified by the team.

At the end of each period of operation performance summaries are returned to each group. An income statement is provided which gives information on revenue from sales of "D" and "C", cost of material sold, gross profit on sales, operating expenses (including plant depreciation), general expenses (including inventory charges and R&D expenditures), interest from unspent funds, and net profit. A balance sheet lists the company's current assets, plant and equipment, and liabilities and equity. In a marketing report the market fractions of "D" and "C" captured, the product selling prices, product costs, and the amount of product produced in inventory and sold are reported. Operating conditions for the year are listed in a plant operations report and an R&D status report is given. This includes a projection of the year in which the sale of "C" will begin (at the 95% confidence level) if a program has been initiated, and the plant is operating efficiently. These reports are treated as proprietary for each company. In addition to supplying essential information, these reports provide experience in analyzing accounting statements.

Production facilities may be expanded at the beginning of Year 5 if sufficient funds have been generated from the sale of the primary product "D" and possibly the sale of "C" resulting from a research breakthrough. Design specifications for any expansion (consistent with the available funds) are submitted for the beginning of Year 5. Increased production will begin in Year 5 so that increased sales can contribute to the revenues reported for the fifth year. The simulation is repeated through Year 10. The performance of each group is evaluated on the basis of the return generated from the initial $9 million investment.

Progress toward the R&D breakthrough is determined by a Monte Carlo procedure which operates by sampling at random, but with the frequency of a "research probability function."

CLASS EXPERIENCE

The simulation has been performed at various stages of evolution six times in the course CHE 691, Technical Project Management, offered in the Department of Chemical Engineering at the University of Delaware. The current form has been used for three classes of CHE 691 and has been tested in three additional exercises with volunteer groups. Student time to complete the game varies from 25 to 35 hours and some 3 to 5 hours are required for class discussion and presentations. The results summarized in Tables 1 through 3 and Fig. 3 are typical results from a simulation carried out in the fall of 1978.

The plant capacities specified by each team before and after expansion are summarized in Table 1. In this particular simulation two teams (III and IV) elected to pursue the R&D programs for the commercialization of the by-product "C" while teams I and II built large production facili-

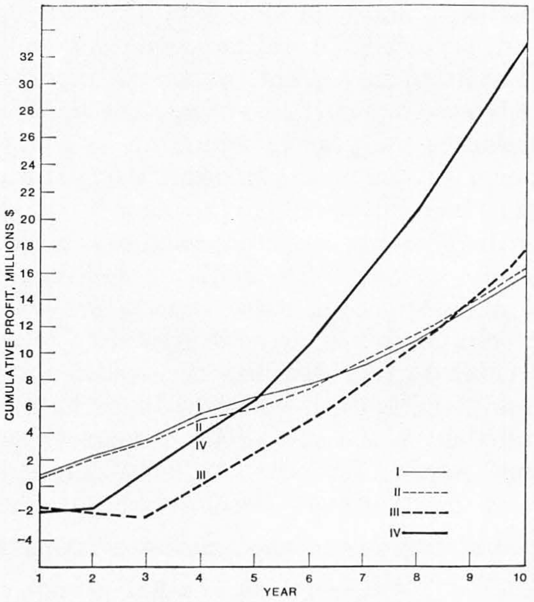


FIGURE 3. Trends in cumulative profit over the ten-year game.

ties in an effort to capture the established market for the primary product "D". The initial production capacities of the teams conducting research were about 40% smaller than the teams that declined the research program.

Team I elected to build a large capacity distillation column in order to insure flexibility of production rates. Due to the high cost of the column relative to the reactor, they were forced to construct a smaller reactor to stay under the $9 million limit. Team II also elected to construct an oversized distillation column. Team III constructed a more modest column which could handle a flow 20% in excess of the optimum flow rate. Team IV tightly designed the distillation column to match the optimum flow rate from the reactor.

The teams that elected not to support the R&D program designed their processing units to provide about 40% of the projected demand for product "D" in Year 3. Teams III and IV built the maximum capacity facilities possible with the funds remaining after the commitment to the R&D program.

The sensitivity of the outcome shown in Fig. 3 to competitive interactions is illustrated by the results summarized in Tables 1 through 3. Teams I and II built large production facilities by foregoing research. As a result, they captured a large percentage of the market for product "D" and acquired relatively high cumulative profits during the first three years while Teams III and IV carried out product "C" research. When Teams III and IV made product "C" research breakthroughs in Year 3, their profits began to swing upwards from the increased revenues. Team IV went on to accumulate the most profit by a great margin

TABLE 1
Summary of Facilities

INITIAL	I	II	III	IV
Reactor Size, in m^3	**45.1**	**50.0**	**50.3**	**50.5**
Reactor Cost, in \$ x 10^6	**1.74**	**1.91**	**1.92**	**1.93**
Distillation Column Design Limit, in Kg-"D"/yr x 10^5	**6.7**	**5.6**	**4.2**	**3.8**
Distillation Column Cost, in \$ x 10^6	**6.79**	**5.89**	**4.94**	**4.64**
Initial Capital Investment (year 1), in \$ x 10^6	**8.53**	**7.80**	**6.86**	**6.57**
R&D Investment (year 1), in \$ x 10^6	**0.00**	**0.00**	**2.00**	**2.00**
Maximum Capacity, in Kg-"D"/yr x 10^5	**6.7**	**5.6**	**4.2**	**3.8**
EXPANSION				
Reactor Size, in m^3	**45.1**	**67.5**	**30.2**	**54.6**
Reactor Cost, in \$ x 10^6	**1.74**	**2.50**	**1.22**	**2.07**
Distillation Column Design Limit, in Kg-"D"/yr x 10^5	**6.7**	**6.6**	**2.2**	**6.8**
Distillation Column Cost, in \$ x 10^6	**6.79**	**6.34**	**3.50**	**6.64**
Total Capital Investment in Expansion (year 5), in \$ x 10^6	**8.53**	**8.84**	**4.72**	**8.71**
Overall Capital Investment in Equipment, in \$ x 10^6	**17.06**	**16.64**	**11.58**	**15.28**
R&D Investment (year 1), in \$ x 10^6	**0.00**	**0.00**	**2.00**	**2.00**
Total Maximum Capacity, in Kg-"D"/yr x 10^5	**13.4**	**12.2**	**6.4**	**10.6**

TABLE 2
Distribution of Market Share (%)

Period (Year)	"D" Team I	II	III	IV	"C" Team III	IV
1	31	30	19	20	—	—
2	35	30	14	21	—	—
3	37	30	12	21	15	85
4	35	29	16	20	53	47
5	34	30	16	20	45	55
6	28	31	17	24	37	63
7	29	30	15	26	37	63
8	31	29	15	25	37	63
9	32	28	15	25	37	63
10	32	28	15	25	37	63

by the end of the simulation. This one-sided outcome was due in part to mistakes in judgment made by the other teams.

Team III did not initiate a "crash" research program until the second year; nonetheless, they managed to achieve a "breakthrough" in the same period (Year 3) as Team IV (Table 2). Unfortunately, Team III did not anticipate such an early breakthrough and had not built up sufficient inventories of "C" by storing product made in prior periods. Consequently, Team IV captured 85% of the "C" market in Year 3 simply because they had the product available for sale. Team III responded by increasing production to generate more "C" (Table 3). At this point both Team III and IV began to view product "C" as their primary product with "D" relegated to the role of a by-product. Table 2 shows the results of this strategy.

Team III's fear of high inventory cost is reflected in their production strategies for the primary product "D". The mandatory accumulation of inventories of "D", that resulted from the small market share (19%), contributed to a deficit of $1.6 million for Team III in period 1. In order to avoid additional inventory costs, they drastically reduced production in Year 2 (see Table 3). This caused a further decline in the market share for "D" that led to a cummulative deficit of $1.9 million. As shown in Table 3, Team III increased production slightly in Year 3. Shored up by the breakthrough into the "C" market, Team III became more aggressive in Year 4. Unfortunately for Team III, the past production strategies left them with inadequate funds for a significant expansion in Year 5 so that Team IV gained and maintained control of the "C" market for the remainder of the simulation.

Team I elected to allocate all the available funds to the construction of facilities for the production of the primary product "D". The decision to build an oversized distillation column to provide flexibility in operation introduced a significant penalty by reducing the funds available for the construction of the reactor. As a consequence, Team I had the largest capability for producing "D" but was penalized by having the smallest reactor (see Table 1). The small reactor led Team I to operate at a conversion of 71%—well below the optimum conversion of 85%. Team II also emphasized flexibility in operating conditions by building an oversized column which they consistently operated at an off-optimum conversion of 78%. Neither Team I nor II used the flexibility in production rates that had been so dearly purchased. Both teams tended to operate at the non-optimal maximum production rate throughout the simulation. This operating strategy led to a reduced return on the capital investments. In order to meet demands, all teams ran their facilities at the maximum production rate in the latter periods of the simulation.

Team IV operated close to the optimum conversion level consistently and stored a large amount of by-product "C" in inventory in anticipation of a research breakthrough. This strategy gave them the highest cumulative profit at the end of the simulation. However, had Teams I and II operated their facilities closer to optimal and had Teams III and IV been in closer competition

TABLE 3
Summary of Operating Strategies

Period (Year)	Conversion (%) I	II	III	IV	Production of "D" (kg/yr x 10^5) I	II	III	IV
1	75	78	86	85	5.8	5.5	3.5	3.8
2	71	″	93	″	6.7	″	1.8	″
3	71	″	91	″	6.7	″	2.3	″
4	71	″	84	″	6.7	″	4.2	″
5	71	″	84	″	6.7	″	4.2	″
6	80	″	84	″	4.7	″	4.2	″
7	71	″	84	″	6.7	″	4.2	″
8	71	″	84	″	6.7	″	4.2	″
9	71	″	84	″	6.7	″	4.2	″
10	71	78	84	85	6.7	5.5	4.2	3.8

Continued on page 87.

cern here belongs to the energy transported by conduction per unit area across an area located at **x** and normal to **n**, denoted by $q(\mathbf{x},t;\mathbf{n})$. The first law of thermodynamics applied to volume V bounded by A, gives

$$\frac{d}{dt}\iiint_V [\hat{u} + \frac{1}{2}v^2]\,dV + \iint_A [\hat{h} + \frac{1}{2}v^2]M_j\,dA_j = \iint_A dA_j T_{ji} v_i + \iiint_V \rho f_i v_i\,dV - \iint_A q(\mathbf{x},t;\mathbf{n})\,dA \tag{12}$$

The interpretations of the various terms in Eq. (12) are available in any standard textbook. In view of the pattern already set before we are able to conclude that

$$\lim_{V\to 0}\frac{1}{A}\iint_A q(\mathbf{x},t;\mathbf{n})\,dA = 0$$

so that there exists an energy flux vector $[Q_j(\mathbf{x},t)]$ such that

$$q(\mathbf{x},t;\mathbf{n}) = n_j Q_j(\mathbf{x},t)$$

or

$$q(\mathbf{x},t;\mathbf{n}) = \mathbf{n}\cdot\mathbf{Q}(\mathbf{x},t)$$

Thus the conservation principles are themselves responsible for "fluxes" being vectors or tensors, a result of tremendous significance in the investigation of the mechanics of continua. It is a fact that deserves mention in courses on fluid mechanics and transport phenomena.

ACKNOWLEDGMENT

Personal discussions have borne out that the issues raised in this paper are a routine matter to many. The authors would like to specially acknowledge Professors L. E. Scriven at the University of Minnesota and Stephen Whitaker at the University of California, Davis. In particular, Professor Whitaker was kind enough to provide evidence that the contents of this paper are not common knowledge and represent useful information. ☐

COMPETITIVE ENVIRONMENT

Continued from page 81.

for product "C", Team II could have gained the largest profits.

Upon the completion of 10 operating periods, a year by year summary of the performance of all teams is made available to the participants. Each team is asked to prepare a report to analyze their performance and identify the important decisions and actions that led to their relative position in the competition. Although the simple "return on investment" is suggested as a possible economic evaluator of performance, the teams are at liberty to select alternate evaluators; e.g., "internal rate of return" (the interest rate that makes the cumulative discounted cash flow equal to zero) or "borrowing power". As would be expected, those groups that make significant profits in the early periods of the simulation tend to base comparisons on the "internal rate of return". The use of these alternate measures of performance can cause reversals in the relative positions established by comparisons based on "net profit" or the simple "return on investment" criteria.

CONCLUSION

Student response to this project has been enthusiastic. The immediate consequence of their decisions provides a sense of realism for the interplay between technical, marketing, and economic factors. The computer simulator, the package of memoranda, and instruction manual are available at a total cost of $275.00 from Engineering Educational Materials, 805 Baylor Drive, Newark, Delaware 19711. ☐

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