

THE INDUSTRIAL PRACTICE OF CHEMICAL PROCESS ENGINEERING

S. W. BODMAN

THE MIT PRESS CLASSICS

The Industrial Practice of Chemical Process Engineering

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Preface

With study of the engineering sciences now a dominant factor in the curricula of many academic engineering departments, only limited time is available for the creative application of theoretical fundamentals to practical chemical processing problems. In particular, the study of process design and financial evaluation is often either disregarded or given only cursory attention. As a result, the young engineering graduate frequently encounters difficulties in becoming acclimated to the environment of a commercial organization and in maximizing the benefits which can be generated from his technical background.

In order to prepare its students more fully for the challenges of industrial work, the M.I.T. Chemical Engineering Department has developed two specific programs. First, the department's School of Chemical Engineering Practice exposes graduate students to actual problems in an industrial environment under the direct and close supervision of a faculty member. This program has been in operation for over fifty years and has proven to be an effective contributor to a student's total academic experience. To complement the Practice School program, a senior-year synthesis course in process design has been developed. Professor Thomas K. Sherwood summarized his original work in the development of the M.I.T. process design course in his text "A Course in Process Design". The course, as conceived by him, is based upon a series of design cases; for each case the student is required to devise and analyze process schemes that might lead to the solution of the design problem.

The present text seeks to combine some aspects of the Practice School program with elements of Professor Sherwood's case-study approach to instruction in engineering design. It is hoped that the result of this combination will not only be useful as a text for academic process design instruction but will also serve as a reference book for the young engineer embarking on a career in industry.

An introductory chapter briefly describes the interaction and interdependence of market research, process design, and financial evaluation functions in commercializing a chemical product. Methods of planning and analyzing laboratory experiments, of utilizing market and financial information, and of preparing and presenting a chemical process design are discussed. The introduction is followed by a series of six case studies in engineering design, typical of those encountered by a young engineer in his initial industrial assignments. The need for accurate analysis and correlation of laboratory data is given great emphasis. Secondly, the need for devising creative and practical solutions to processing problems is given some discussion. Finally, each case illustrates methods of combining technical and financial information to provide a realistic evaluation of a proposed process. Each case is concluded with a recommended design as well as suggestions for further work that would be required in subsequent, more detailed, design efforts.

A great deal of emphasis has been placed on the use of the digital computer in the analysis and presentation of design problems; computer programs are presented for three of the cases discussed. These programs and others like them have proven to be particularly stimulating when used in a "computerized classroom," wherein the student can communicate directly with the machine. In preparing portions of the text, it has been assumed that the reader has at least some knowledge of the FORTRAN coding language.

The present volume was written while the author served as Director of the Bound Brook Station of M.I.T.'s School of Chemical Engineering Practice. This station is located with the Organic Chemical Division of the American Cyanamid Company, Bound Brook, New Jersey. The data used in the preparation of Chapter 3 were gathered by a student group as a part of a project at the Bound Brook Station. The author is grateful to American Cyanamid for its permission to use these data as well as for the company's hospitality during the 1965-66 and 1966-67 academic years.

Many individuals have contributed substantially to the case studies summarized in this book. First of all, thanks are due to Professor Thomas K. Sherwood, who has continued his guidance in the instruction of chemical process design at M.I.T. It was he who originally suggested the preparation of the present text, and Chapters 2 and 4 are based almost entirely on design cases developed by him for his process design courses. Sincere appreciation is expressed to Professor Robert York of Cornell University for his guidance in the economic evaluation of chemical projects and for his instructive review of portions of the present text. Professors C. J. King and Scott Lynn of the University of California in Berkeley were kind enough to review the entire text of this book. Their comments were particularly significant in giving additional breadth and meaning to several of the case studies. Dr. Howard Kehde and his colleagues at Dow Chemical Company, Midland, Michigan, very kindly reviewed the cases concerned with styrene production; their comments provided an invaluable dimension to those cases by bringing to bear the knowledge and sophistication of a major producer of styrene monomer. Professor Giles R. Cokelet of California Institute of Technology provided a valuable commentary on the sulfur transportation case. Professor R. G. Thorpe of Cornell University originally acquainted the author with some of the difficulties

associated with the vacuum fractionation of styrene-ethylbenzene mixtures; this information was most useful in the preparation of Chapter 6. The data used as a basis for Chapter 3 were gathered under the direction of Professor Michael Modell of M.I.T.; his cooperation in making this information available is greatly appreciated. Several former teaching assistants and students at M.I.T. contributed substantially to the development of computer programs for Chapters 5, 6, and 7. In this respect, special thanks are due to Robert L. Blumberg, Bruce Crocker, Avelino R. Rodriguez, and Robert L. Sandel.

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1. Introduction

The industrial practice of chemical engineering design requires the application of many talents and skills. By the definition of his profession, the process design engineer in the chemical industry implements the work of the chemist and development engineer in providing mechanical and structural specialists with a realistic description of the required equipment. Sherwood (44) has recently described the following functions which must be performed to span the gap between bench-scale chemistry and the operating plant:

1. Recognition of an economic opportunity
2. Conception of a plan or design
3. Preliminary analysis of the design
4. Completion of a final design
5. Implementation of construction and operation

These functions are useful indicators of the stages through which a design must pass and of the various scales of thinking which are required of the design engineer. The foregoing list is quite helpful in placing each individual job in the perspective of the over-all effort which is required. In the analysis of a design project, it is to be remembered that an economic evaluation for the entire project must be completed after each step in the design; in the absence of a favorable evaluation after each step, the time and effort required by the next step cannot be justified.

To complete the transition from laboratory conception to operating plant successfully, the design engineer in industry must call upon a wide background not only of technical fundamentals but also of financial and social understanding. For example, knowledge of geographical factors may be important in selecting a proper plant site, while a grasp of corporate finance and economics may be a prerequisite to a proper evaluation and presentation of the economic benefits to be gained from a specific chemical project. Clearly an understanding of the operation of modern computation equipment is now an essential part of the training of a design specialist. In addition to having a

broad technical background, the successful design engineer must continually develop talents in analyzing his own technical performance and in evaluating the efforts and contributions of other people.

The present text describes the type of technical and economic background necessary for the successful completion of a chemical process design. These fundamentals will be summarized briefly in the present chapter. This introduction is followed by a series of design case studies that serve to illustrate important aspects of industrial chemical engineering design.

The cases selected for presentation illustrate not only different types of engineering projects but also variations in the required degree of completion for a design. Cases requiring chemical reactor design, separation equipment design, and pipeline sizing and optimization are included. One of the most difficult aspects of these design cases, or for that matter of any realistic technical problem, is that of defining the real nature of the problem, i.e., deciding what is required. One of the more common failings of a technical program results from a tendency to answer a question that has not been asked or to complete work that has not actually been requested. This difficulty is particularly prevalent in design work, where many different types and degrees of effort may be required. The case studies here presented illustrate industrial problems and are summarized in the form of memoranda. In some instances the data were obtained from the literature, while other cases represent actual industrial problems where the data originated in a company laboratory and where the indicated result constitutes the actual solution presented to management.

In each of three cases cited, the design analysis is summarized in the form of a computer program which is reproduced in the text. Results generated by each program are employed to evaluate the economics of a design as a function of the important process variables. However, results for all possible combinations of these variables have not been obtained, and the computer programs are presented in order that they may be further exploited to refine the economic evaluation of the projects to which they apply. These programs have been found particularly useful when applied in a computer classroom—a situation in which a class can "communicate" directly with digital computation equipment.

The use of a computer to evaluate in detail a chemical process represents one extreme of the situations that might be encountered by a typical industrial design group. At the other extreme is the situation where no detailed design or economic evaluation is required and only a modest number of calculations is needed to establish the most likely configuration for the ultimate design. In the cases of the latter type which are presented in this volume a consideration of limiting cases and the use of shortcut methods in preparing the calculations prove to be most helpful.

By presenting a series of cases having not only a varied technical content but also a varied degree of required sophistication, this text attempts to illustrate some of the concepts associated with the suc-

successful completion of an industrial process design. By definition, process design is involved with the application of technical principles to the available experimental information in order to produce a workable manufacturing process. As such, design cases have traditionally been examined individually with relatively little emphasis on a consistent set of principles necessary for the proper understanding and successful execution of general classes of problems. To some degree, such a set of principles can be established; as a guide in making the ensuing case studies meaningful beyond their own particular boundaries, the following set of principles may be considered:

1. Determination of design requirements
2. Comprehension of market conditions
3. Evaluation of experimental data
4. Establishment of critical design parameters—simulation and optimization
5. Evaluation of process economics
6. Presentation of design results

The present introduction does not purport to be a thorough review of each subject listed. Only a cursory discussion of each point is offered, together with a review of a few pertinent references. Neither should the reference citations mentioned be considered as a complete literature review; they are merely those that have proved useful in working with young chemical engineers encountering their first industrial design problems.

DETERMINATION OF DESIGN REQUIREMENTS

The sophistication of a process design must be tailored to meet the requirements of the individual situation. As mentioned before, the use of data-processing equipment allows the designer more freedom than ever before to investigate various combinations of system parameters. Indeed, one of the major functions of the present text is to demonstrate the utility of machine computations in studying various aspects of a process design. Nevertheless, the advent of modern computers makes it quite easy for the user to pass through the point of diminishing returns. A great deal of objective thinking is required to avoid solving problems merely for the intellectual satisfaction gained from the solution. As in all aspects of engineering for industry, if the value of the programming and computer time used is not exceeded by the value of the design improvement gained, then both engineering and computer time have been misspent.

To determine the possible need for a detailed design calculation, it is most useful to analyze limiting aspects of a design situation by means of simple hand calculations. Computations for limiting cases

are often quite straightforward, since simplifying assumptions can usually be made. For example, if a laboratory reactor has been operated adiabatically between two temperature levels, the results of such an experiment can be scaled directly to a commercial-scale adiabatic unit operating between the same two temperature levels. Comparison of this result with that obtained by assuming an isothermal operation at the lower temperature level sets the extremes between which nonisothermal designs must fall. By noting the variations in the important design parameters as the design is shifted from one limit to another, one can assess the need for making more detailed and often more time-consuming calculations at intermediate conditions. Such a calculation procedure is illustrated by Chapter 4, in which a reactor for the hydrogenation of benzene is designed. The need to make a comparison of limiting conditions would seem obvious; nevertheless, this simple technique is often overlooked, resulting in an unnecessary expenditure of engineering and/or computer time.

One of the most valuable talents that can be developed by the design engineer is an ability to perform the simple calculations necessary to establish the limiting cases of a design, where the most difficult technique is often that of making the appropriate assumptions in order to simplify the calculations. This ability usually must be developed through many years of experience, and the novice often finds it quite difficult to achieve. It is to be appreciated, however, that the ability to perform a simple but meaningful analysis of a problem does not develop automatically with experience. A conscious effort must be made to compare the results evidenced in the final operating plant with the assumptions made in the early stages of the design. Only by such a feedback and by comparison can the quality of subsequent estimates be upgraded.

The need for limiting-case calculations cannot be overemphasized; such calculations should be applied as early as possible in the consideration of any chemical project. More and more effort is being made today and will be made in the future to provide the research manager with a quantitative estimate of the probability for the technical and economic success of a particular research project. Clearly a major ingredient in such an estimate must be a preliminary forecast of the capital and operating costs for the project. This type of estimate is necessarily based on little or no data, and the computations must result from some sort of limiting-case analysis. Thus the ability to perform such an analysis is valuable not only in establishing preliminary limits on the process variables but also in determining whether the probability for financial success justifies the expenses involved in the bench-scale and pilot-scale experimental work.

In this light, the design engineer should enter into consideration of a chemical project at the bench stage. If his initial calculations do not show a high probability for financial success, the very existence of the bench work should probably be reconsidered unless external circumstances, such as a raw-material position, are more important than economic factors. Similarly, as work proceeds through bench and pilot-scale development, discussions between development groups and a process design engineer may be very important, particularly in

coordinating technical progress with the efforts of market research groups.

COMPREHENSION OF MARKET CONDITIONS

Cooperation between the design engineer and the market research and development groups is of critical importance. One of the most essential pieces of information required for the completion of process design calculations is an estimate of both present and future market demands for the product under consideration. In many cases the ability of a design engineer to analyze technical information and to provide an accurate scale-up to commercial equipment will have only a modest influence on the economics of the final operating plant. On the other hand, an accurate sales forecast for a product is usually quite critical to a realistic prediction of the ultimate financial performance of the operating unit.

For example, a 20 per-cent error in a kinetic constant or heat-transfer coefficient may be damped out at that stage in the calculations in which the over-all process economics are considered. However, a similar percentage error in a market forecast may well be amplified as it is transmitted through the calculations leading to an economic evaluation of the project.

Sources of market information run all the way from government reports to the annual reviews published by the various trade journals. Most important, however, are the personal discussions of salesmen with customers, and it is this type of interaction which forms the best basis for sales forecasts. Typically, the sales forecasts will be prepared in the very early stages of process development, but they are subject to rapid and substantial deviations as the market research work proceeds. It is essential that the process design group be continually kept informed on the status of the market estimates. Only in this way can a final design be produced which will be justified by present and future market estimates. Finally, it should be remembered that plant construction is usually finished two years or more after the design plans are completed. If economic conditions are favorable, the need often arises to expand the plant facilities even before construction is complete. This factor further emphasizes the need for accurate market forecasting procedures.

Because of the difficulty in gathering and processing meaningful raw data, the chemical engineering literature has historically given only scant attention to the subject of marketing. More recently, the availability of the electronic computer has made feasible the collection and assessment of market information sufficiently broad and accurate to allow the development of useful marketing theories as applied to the chemical industry. A corresponding increase in research and publication activity in this area has been evidenced. Of particular note is a series of papers presented at a 1965 American Institute of Chemical Engineers symposium in which the interaction of research, marketing, and design efforts was discussed (9, 11, 13, 24, 42). These papers were prepared by men familiar with all aspects of product

commercialization in the chemical industry, and the series provides an excellent exposition of the advantages to be gained and the problems encountered by efforts to coordinate marketing and research programs. The papers are particularly valuable in illustrating the various methods by which an engineer can assure that an adequate market picture will be obtained and that a correspondingly accurate financial evaluation will be achieved. Another compendium of papers dealing with chemical marketing has been published by the American Chemical Society (1). This book, which contains twenty contributions, serves as an excellent background source for the specialized areas of marketing. For example, the roles of product advertising, applications research, and product delivery methods are given detailed treatment.

There is a very definite need for a complete review of recent chemical marketing literature. Such a review, preferably carried out by someone with a strong background of industrial marketing experience, would not only clarify the situation for the student but would also hopefully lead to better market analysis techniques for the industry as a whole.

EVALUATION OF EXPERIMENTAL DATA

In the manufacture of a particular chemical, the required process steps generally follow the sequence shown below:

1. Preparation of reactants
2. Carrying out of reaction(s)
3. Heating or cooling of reaction products
4. Separation of reactants from products and purification of products

Almost without exception, the design engineer is required to base his analysis of each step upon laboratory data generated by other investigators or obtained from the literature. For those having only a modest exposure to the chemical literature, Mellon (32) has provided a very useful guide to the proper methods to be used in searching the literature. In using literature data for the engineering analysis of a process operation, it is critical to develop an appreciation for the quality of the information to be used. For example, data reported many years ago may have been obtained before sufficient theory had been developed to allow a proper analysis and presentation of the experimental information. In the absence of such a theory, early experimenters sometimes failed to measure a variable necessary for proper analysis. Obviously, the experimental equipment available in the early engineering laboratories was not as sophisticated as that currently available; it is therefore important to develop an appreciation for the strengths and failings of various types of laboratory apparatus.

Difficulties with the proper interpretation of published data are frequently compounded by industrial censorship of process information. The suppression of technical information is obviously necessary

to protect the commercial value of a process. However, from a technical viewpoint, censorship often requires the engineer to make a "reasonable" assumption in order to be able to proceed with his analysis.

A good example of the censorship of industrial information is provided by MacMullin (30), who discusses the distribution of reaction products for the chlorination of benzene. He presents data that establish the distribution of the various chlorinated compounds as a function of the total amount of chlorine reacted. This information is of course not sufficient for the design and evaluation of a manufacturing process, since the kinetic parameters for the reactions are not disclosed. In order to complete a design, reasonable values of the chemical kinetic constants must be assumed; such a procedure was followed in preparing Chapter 2, in which various processes for the chlorination of benzene are discussed. When it is necessary to proceed in this manner, it is most desirable to obtain literature information from as many different sources as possible. By comparing and combining all available information, one is often more likely to establish a realistic basis for a design. In fact, the technique of gathering and comparing information from a number of sources is frequently useful in many aspects of a process design.

Before investing the time and effort required even by a preliminary design calculation, it is prudent to assess the validity and consistency of the laboratory findings upon which the design is to be based. This assessment is most easily accomplished by comparing the data directly with appropriate literature information. For example, the general accuracy of a set of vapor-liquid equilibrium data for a mixture of two components may be checked most directly by comparing them with those for the same two compounds but for other conditions of temperature and pressure. If such data are not available for the desired compounds, the relative volatility computed from the laboratory result might be compared with that calculated for an ideal mixture by using Raoult's law. It may also be informative to compare the relative volatility with that for other compounds having similar chemical structures. Finally, the thermodynamic consistency of the data should be assessed by invoking one form of the Gibbs-Duhem equation.

Similarly, by plotting the observed solubility of a solid in a liquid versus the reciprocal of absolute temperature on semilog paper, one should obtain a straight line from whose slope the heat of solution can be computed. A comparison of this heat of solution with heats of solution or heats of fusion for chemically similar compounds yields a check on the validity of the experimental data. An analogous technique applied to chemical kinetic data or chemical equilibrium data would yield an activation energy or a chemical enthalpy change that could then be compared with literature values.

Table 1-1 has been prepared to summarize the methods for assessing the validity of those types of data most often encountered in completing design projects for the chemical process industries. It is to be emphasized that this table is not a summary of design methods but merely a set of criteria by which to judge the quality of technical

data to be used in carrying out a design. The references shown are not meant to be comprehensive; moreover it is clear that the table vastly oversimplifies the types of operations carried out in the chemical industry as well as the theoretical and technical background necessary for the completion of even a simple design problem. Nevertheless, the information summarized has proved very useful in applying the results of theoretical considerations to engineering problems of practical significance. Naturally, in many instances it is both desirable and necessary to supplement the elementary methods described in Table 1-1 by using some of the more advanced theoretical developments.

The utility of the information summarized in Table 1-1 naturally varies significantly from one segment of the chemical process industry to another. For example, the organic chemical industry makes great use of extraction and leaching processes, and the simple technique of plotting solubility data on semilog paper to obtain a heat of solution can prove to be of great and frequent utility. Once confidence in the experimental data is developed, the design calculations to optimize the number of extraction or leaching stages can proceed quite smoothly.

When theoretical correlation of process information is impossible, the use of a factorially designed experimental technique may be of great value. The use of statistically designed experiments is particularly valuable in reducing the required amount of experimental and analytical effort to solve a problem for which there is little or no theoretical basis. The following references, arranged by Koehler, provide an excellent introduction to the application of statistical concepts to a variety of problems encountered in the chemical industry. Besides a discussion of statistical designs in the analysis of laboratory and pilot plant data (7, 23), the series also effectively presents the advantages to be gained by the application of statistical techniques to in-plant experimentation (22), to the use of computers in data reduction (41), to the selection of appropriate production-line control charts (17), and to the general improvement of quality-control methods (26). When a sound theoretical basis for a process design is limited, the use of statistical methods can provide a highly useful foundation for the necessary design and evaluation calculations.

One last point frequently overlooked is the need for preparing an adequate error analysis. If the probable error as computed for the experimental technique used is approximately equal to the random deviation of the data about a correlating line, then it can be assumed with a high degree of confidence that all sources of error have been properly established and accounted for. Such an analysis lends a great deal of confidence to the use of the data in a design, particularly when the expenditure of a large capital investment is required.

ESTABLISHMENT OF THE CRITICAL DESIGN PARAMETERS— SIMULATION AND OPTIMIZATION

In his text, Sherwood (41) states quite appropriately that the designer must be willing to make assumptions. Once sufficient informa-

Table 1-1. Useful Methods of Evaluating and Correlating Chemical Engineering Experimental Data

Process Operation	Required Design Parameter	Bases for Evaluation or Correlation of Data	Literature References
Fluid transportation	Friction factor	$f/2 = F(N_{Re})$	(34)
Fluid heating or cooling	Heat-transfer coefficient	$j_H = F(N_{Re})$	(31)
Chemical reaction	Chemical-kinetic constant	Arrhenius correlation	(46)
	Chemical-equilibrium constant	van't Hoff correlation	(52)
Catalytic chemical reaction	Effectiveness factor	Thiele modulus	(40)
	Mass-transfer coefficient from fluid to catalyst pellet surface	$j_D = F(N_{Re})$	(40)
Slurry reaction	Mass-transfer coefficient from liquid to catalyst pellet surface	$k_L = F(D, N, D_p, \mu, \Delta\rho)$	(49)
Sparged reaction	Mass-transfer coefficient at the bulk liquid surface	$k_L = F(D, N)$	(27)
Absorption	Mass-transfer coefficient from a gas bubble to bulk liquid	$k_L a = F(D, N, V_g)$	(45)
	Solubility of gas in a liquid	Henry's law or Raoult's law	(21)
Boiling or condensation	Vapor pressure	Clausius-Clapeyron equation	(52)
Distillation	Vapor-liquid equilibrium (relative volatility)	Gibbs-Duhem equation	(37)
Crystallization	Tray efficiency	Murphree efficiency relationship	(37)
	Solubility and supersolubility	Clapeyron-type correlation	(14)
Extraction	Distribution (partition) coefficient	Nernst's law	(14)

tion is available to analyze a process completely and accurately, typically the financial incentive for completing the design will be substantially diminished. However, in order to make appropriate preliminary assumptions, the designer must develop the capability of isolating the variables that are critical to the determination of the over-all economic performance of the process. Frequently a preliminary design calculation is required to establish the identity of the most important design variables. Such a case is illustrated in Chapter 4, in which the hydrogenation of benzene is considered.

For the more common process operations, the critical variable frequently is well known; e.g., in the design of a distillation column, the reflux ratio usually serves as a most sensitive index of the process economics. In the first analysis of a unique or a highly complex design, the determination of the most critical variables often is left to the judgment of the engineer. Typically, when a multivariable design is approached, a base case is selected by arbitrarily establishing "reasonable" values for many of the process variables that are believed to be least critical in determining the process economics. The variables thought to be most critical are allowed to vary, and a preliminary economic evaluation and optimization of the design are completed. Then variations from the base case are considered by allowing variations in the parameters that had previously been fixed. As shown in Chapter 7, in which the economics of styrene production is considered, the use of a digital computer can greatly facilitate the evaluation of the base case and the variations from this case that are significant. As illustrated in the same chapter, it is essential to return to the original set of assumptions in order to establish the effect of each assumption on the over-all economics of the process. It is also important to realize that in dealing with a multivariable design problem, several local minima may exist; a certain amount of judgment must be exercised in determining whether a local or an over-all minimum has been achieved.

The calculation procedure described suffers from the lack of an organized approach to the problem, and a great many decisions must be reserved for the judgment of the engineer. In certain types of design problems, a more quantitative approach to the logic required for a design calculation may be achieved by applying the technique of linear programming. This method has application in design cases that result in linear algebraic relationships. Happel's very useful text on chemical process economics (18) includes a brief description and an example of linear programming techniques. It is important to note that many chemical economics problems are highly nonlinear and that in such instances linear programming techniques are not directly applicable. However, by linearizing the appropriate analytical expressions, linear programming techniques may be helpful in establishing the general nature and relative importance of the cost functions under study.

A significant portion of modern chemical engineering research has focused on the development of advanced methods for process optimization as applied to individual sections of a process as well as to the over-all design result. Particular emphasis has been placed

on the optimization of chemical reactor systems; much of this work is well summarized by Aris (5, 6), Denbigh (15), and Kramers and Westerterp (28). One of the more important of modern optimization techniques is that of dynamic programming, in which the last of a series of staged operations is first optimized; the last two stages are then optimized as a single unit. One stage is added on in a stepwise fashion, working backward until the optimum conditions for the entire process are established. This method has obvious application in the analysis of continuous stirred-tank reactor systems (5). The calculus of variations has been shown to have particular value in the optimization of tubular reactors; the method is especially useful in the case of adiabatic reactions (15). In addition to the aforementioned, the method of "steepest ascent" has also proved useful in the optimization of reactor systems (20). This technique allows one to approach an optimum as closely as desired by successive quantum changes in the process variables until the design parameter in question (e.g., yield) is optimized.

Concurrent with the development of optimization methods has been the establishment of new techniques to simplify and minimize design computational effort. Rosen (38) has presented a machine computation method for performing process material balances, and Ravicz and Norman (36) have reported a more flexible program incorporating both heat and material balances. Sargent and Westerberg (39) have developed a general-purpose approach that is very helpful in organizing the programming work required for the computer simulation of a chemical process.

More recently, Lee, Christensen, and Rudd (29) have made a very significant contribution in the study of multivariable design problems where assumptions are required to proceed with the design. These investigators have established a method that allows the preassignment of values to a selected set of design variables in such a way as to minimize the computational effort. This work is one of the first signs of a trend in the chemical engineering profession to make more effective use of computers in the analysis of process design problems.

EVALUATION OF PROCESS ECONOMICS

When the chemist undertakes a fundamental research project in the laboratory, he frequently has only a limited notion of the ultimate applications and possible financial success of his product. This sort of freedom has proved invaluable in developing a creative atmosphere for the development of new products. However, once a chemical project emerges into applied research or development, each subsequent step in the project should be evaluated financially before the work for that stage is undertaken. In this manner, projects having a low probability for an acceptable financial return can be "weeded out" at an early stage, and more technical effort can be applied to developing those products which are most likely to realize the greatest economic return.

One of the critical functions of the design engineer (or any other person responsible for evaluating the process economics) is to keep

abreast of the latest technical developments in a new product and to interpret these developments in the light of their ultimate effect on the profit potential. For example, if the production yield of a new product is increased by carrying out the reaction step in a particular solvent, the cost for separating the product from the solvent must be estimated. It may be that the cost of recovering the product overshadows the savings generated by the use of the solvent. If such is the case, the course of the early process research and development for the product will have to be altered accordingly.

The actual form of a financial evaluation varies widely within the industry; and because of the obvious commercial significance of evaluation techniques, little meaningful information is available in the literature. However, some general references are available which have proved very useful in orienting chemists and engineers to the problems associated with a financial evaluation.

In first approaching an economic evaluation, one of the major difficulties encountered by the technically trained person is that of understanding financial terminology. The work of Beattie and Vivian (10) greatly mitigates this problem; it provides a detailed compilation of the definitions for most terms common to financial analysis as applied in the chemical industry. In addition, the importance of using consistent terminology is well illustrated.

In its simplest form, the financial evaluation of a chemical project provides an estimate of the capital required for the construction of the manufacturing facility and a forecast of the costs required to operate the proposed process. By deducting the total operating costs and income taxes from the anticipated sales revenues, the net operating income for the project can be established. In addition to the annual dollar income volume, profitability may also be expressed as the fraction of the capital investment needed to establish the anticipated return. The philosophy guiding the analysis of corporate ventures in the chemical industry is well summarized in an A.I.Ch.E. publication (2).

Each company has its own peculiar raw-material position to protect, its own process know-how, its own accounting system, and its own plans for future expansion. As a result, the identical proposed project may meet different fates, depending upon the company that considers it. For example, consider an American company that is domestically selling products that are facing competition from identical products manufactured in Europe. The European concern might be accounting for the cost of its goods on an incremental basis, i.e., a basis in which depreciation and overhead costs are allocated entirely to the domestic portion of production while the production designated for export is burdened only with direct expenses. Clearly in such a situation the European firm might find itself in a very advantageous competitive situation even after the transportation costs are taken into account. Thus a difference in cost-accounting techniques can cause a vast disparity in the commercial market place. Similar examples are available where difference in raw-material position and process know-how lead to substantial commercial implications.

Some of the more standard methods which may be used in accounting for chemical project costs are elucidated by several texts (18, 35, 43, 50). It should be noted that each company has its own required minimum return on investment for a project; for obvious reasons these figures are necessarily held in confidence. However, in the absence of external circumstances (e.g., raw-material position), an estimate of 8 to 10 per cent is probably a realistic lower limit on the return on invested capital required for project approval. Much higher return percentages are obviously desirable and are frequently obtained.

The mathematics involved in evaluating the economics of a chemical project becomes quite involved when the current values of the various cash flows into and out of the project are considered. In a significant article, Souders (47) has produced an exemplary discussion of this issue together with an interesting comparison of the effects of various profitability criteria on the ultimate investment decision. For the reader interested in a more complete background in the fundamentals of engineering economics, this paper also includes a short but useful bibliography of definitive works in this field.

One of the great difficulties in providing an accurate financial evaluation lies in the fact that both the market price and the demand for individual products as well as the general development of the national economy are dynamic functions. The financial performance of a plant should be examined as a function of both short-term, high-frequency variations and of long-term, gradual growth or decline in the dollar volume of product sales. Schenk (12) presents a brief discussion and a useful example of such a study. He points out that the economics of a chemical project are most strongly affected by variations in the selling price. Following after the selling price, and in order of importance, variations in the sales volume, sales expenses, and capital investment have been found the most critical factors affecting the return on investment. The need for adequate price and sales forecasting is well illustrated by his discussion. An examination of the influence of variations in selling price, sometimes called a risk analysis, is frequently a required component in the final presentation of the financial evaluation of a new chemical project.

Twaddle and Malloy (19) provide a useful discussion of the effects of long-term demand, selling price, and capacity variations on the economic return to be anticipated for a given chemical project. Various methods of graphically illustrating the economic performance of a plant are well illustrated in this reference. In particular, it is effectively demonstrated that accounting for time variations in demand and price has a dramatic effect on the optimum plant size and may radically influence the decision whether the plant should be built at all.

A major deterrent to the proper financial evaluation of preliminary designs arises from the paucity of reliable capital-cost information for process equipment. Chilton's excellent compilation (12) provides a useful background to the problems of cost estimating and to the proper methods of cost data correlation. The correlations contained in his text are quite adequate for preparing preliminary cost esti-

mates; however, it is recommended that other sources (1, 50) be consulted in order to verify cost estimates. In particular, the price estimates for the larger pieces of equipment should be checked by using two or three different references. When the design reaches its final stages, it is normal practice to contact suppliers in order to verify the estimates for all significant pieces of equipment.

PRESENTATION OF DESIGN RESULTS

Regardless of the quality of the technical work that has contributed to the design and evaluation of a chemical project, the total effort may be valueless unless it is properly presented to those who must make the ultimate investment decision. In particular, the need for lucid technical writing has long been recognized as an important issue, and several excellent texts are available for this purpose (25, 33, 48). Generally, a lack of quality in a technical report can be traced to a lack of effort in preparing and polishing the report rather than to a lack of knowledge of grammar, style, or proper report organization.

Often the results of a technical effort must be presented orally. For the speaker who must summarize a mass of technical information in a short time, the American Institute of Chemical Engineers has prepared an excellent booklet (3) which summarizes the important points to remember in preparing the presentation. It is particularly valuable in pointing out the most effective methods of using slides and other visual aids. The texts of Atwood (8), Flesch (16), and Weaver (51) serve as valuable references to the more general aspects of preparing and executing oral presentations.

SUMMARY

The foregoing sections provide a brief introduction to some of the more important issues that confront the industrial design engineer in the practice of his profession. Some of the points discussed suggest various types of formal training necessary to the successful execution of design work. Other issues suggest specific approaches to design problems which have been found useful. In particular, the appropriate application of electronic computation equipment to aid in the design calculations requires more than ever before the use of engineering talents to comprehend and analyze the computed results. The following chapters provide a series of design case studies wherein the important aspects of industrial design practice are brought to bear on realistic problem situations having commercial significance.

NOTATION

- a Interfacial surface area
- D Diffusion coefficient
- D_p Catalyst pellet diameter

f	Friction factor
j_D	Mass-transfer j-factor
j_H	Heat-transfer j-factor
k_L	Liquid-phase mass-transfer coefficient
N	Rotational speed of impeller
N_{Re}	Reynolds number
V_S	Superficial gas velocity
μ	Dynamic viscosity
$\Delta\rho$	Density difference between solid and liquid

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