Advanced Process Engineering

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13 *Volume 76, 1980*

AIChE *Monograph Series*

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

ADVANCED PROCESS ENGINEERING

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No. 13 AIChE Monograph Series Volume 76

1980

Published by

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

345 East 47th Street New York, New York 10017

American Institute of Chemical Engineers
345 East 47 Street, New York, N.Y. 10017

Library of Congress Cataloging in Publication Data

Fair, James R. 1920-
Advanced process engineering.

(AIChE monograph; no. 13, v. 76, 1980)
1. Chemical processes. I. Title. II. Series: American Institute of Chemical Engineers. AIChE monograph series; no. 13.
TP155.7.F34 660.2'81 80-26283
ISBN 0-8169-0167-8

ISSN 0065-8804

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INTRODUCTION

The chemical process forms the centerpiece of the chemical and petroleum industrial complex. It is not coincidental that this complex, a large and vital segment of the world's total manufacturing business, is called the CPI, The Chemical Processing Industries. Chemical engineers find that much of their career activity is process-oriented, whether it be in plant operations, research, design or product development. New or improved processes, to meet the financial and commercial demands of the business arena, are the continuing goal of practicing engineers. The preparation for the engineers' practice, extending back through the undergraduate curriculum to the introductory courses in mass and energy balances at the university, is process-related, whether it be in the classroom or in the laboratory. Chemical engineers all have an important stake in the process and how it is dealt with over its commercial life span, from inception in the pilot plant or at the bench, to final days before the last shutdown and equipment dismantling.

In this monograph we wish to consider the engineering of processes, with emphasis on how the leading edge of technology might be utilized in improving present practices. We shall take a look at how processes might be designed or analyzed if all the modern tools and approaches are brought into play. Such a situation may seem Utopian to many, and yet it may very well be a state-of-the-art situation that needs identification to a profession that may still employ old art at times, and not very new science at other times. The purpose of this presentation, then, is to define "advanced process engineering" and to show how it might be achieved. Any followup then is incumbent on those wishing to improve the quality of the process engineering steps that indeed lead to superior processes.

I. THE PRACTICE OF PROCESS ENGINEERING

A. Process Evolution

The evolution of a new proces proceeds along fairly traditional lines, as shown in Table 1. In the early stages the "idea" is advanced with elaboration through exploratory experiments in the laboratory and market studies by a business group. Although a certain amount of involvement by Engineering is required, the prime responsibility for this early stage of evalution resides with the operating unit handling the marketing territory involved. As exploratory research and economic feasibility studies emerge, the involvement of Engineering becomes greater, and the *conceptual process design* phase is established. All this activity is part of what is termed *process development*.

When the evolution reaches a point where the decision is to move forward, all indicators for future success being positive, a well-defined *preliminary process design* phase is undertaken. The location of this work within the corporate organization may be in Research and Development (R&D) or it may be in Engineering. For smaller companies there may not be such organizational divisions. The important point is that preliminary process design is a key step in the total evolution of the process. There may be pressures to do it quickly, but under no circumstances must it be done carelessly. For as long as the CPI has been in existence this design step, which in large part defines the ultimate economics of the venture, has been the critical step (even though it has not always been recognized as such).

The cost of preliminary process design is ordinarily charged to corporate expenses, that is, it is not capitalized. Thus, the pressure to minimize the cost, especially if the project is thought to be borderline in its final economic evaluation. It must be emphasized, however, that the results of the preliminary process design, as re-cast in economic terms, determine whether the project is to go forward and a plant is to be built. Overly-conservative design can result in unfavorable economics. Overly-optimistic design can lead to later penalties in the form of additional capital costs, unexpected manufacturing costs and, very possibly, non-competitive process economics. Finally, careless and unenlightened design can lead to the worst of all fates: a plant that cannot be run even to meet the product specification premises. Clearly, the preliminary process design phase is critical, and it may require detailed attention (including mechanical design) at sensitive steps.

The results of preliminary process design go into a document sometimes called a Scope Report (see Table 1). This report is provided to support the request for capital funds and, as indicated earlier, it is based on a compromise between technical accuracy, expensed cost of the work, and time pressures for commercial production. The flavor of this compromise was captured by E. R. Kane, president of the DuPont Company, in an early 1978 address dealing with the impact of regulation on the chemical industry. Pertinent excepts from his address are:

> ....I am referring to the familiar engineering process of "scoping" - fact-finding; data-gathering; examining alternative solutions; and determining, in a precise and disciplined way, the difference between what is desirable and what is attainable....[with respect to regulation] it is the clear responsibility of technically-oriented organizations to marshal and present the facts, so that engineering realities can be incorporated.... [and] engineering know-how must be blended into the mix at every step....(131)

As shown in Table 1, the decision by management to appropriate capital funds leads to *final process design*. This is detailed engineering, with relatively little flexibility for altering process conditions already established. The engineering leads to a series of documents, including the engineering flow diagram (EFD). These documents comprise the familiar "process design package" which will be discussed later. The importance of final design should not be minimized, even though it may involve less of the creative

TABLE 1
STAGES IN THE EVOLUTION OF A PROCESS

Cost category	STAGE	Phase	FUNCTION	PRIME RESPONSIBILITY	PARTICIPATION AMONG ORGANIZATIONAL UNITS
Corporate Expense	idea	Conceptual Process Design Phase	Commercial Development Exploratory Research	Operating Co.	Operating Co: Comm. Devel. Dept. Research Dept. Patent Dept. Engineering Dept.
Corporate Expense	Exploratory	Conceptual Process Design Phase	Product Exploration Research	As Above	As Above
Corporate Expense	Feasibility	Conceptual Process Design Phase	Product Application Research Process Research Process Design	As Above	As Above
Corporate Expense	Development: Design Premises* Tentative Process	Preliminary Process Design Phase	Commercial Development Process Design	Operating Co.	Operating Co.: Comm. Devel. Dept. Research Dept. Process Technology Engineering Dept.
Corporate Expense	Define Project, Prepare Scope Report, Capital Estimate		Engineering	Engineering Dept.	As Above
Corporate Expense	Appropriation Request		Management	Operating Co.	Opg. Co. Management Engineering + other corporate departments
Capitalized Cost	Final Process Design		Engineering	Engineering Dept.	Engineering Dept. Operating Co.: Research Dept. Manufacturing Process Technology
Capitalized Cost	Mechanical Design		Engineering	Engineering Dept.	Engineering Dept. Operating Co.: Research Dept. Manufacturing Process Technology
Capitalized Cost	Plant Construction		Engineering	Eng. Dept., Through Mechanical Completion	Engineering Dept. Operating Co.: Manufacturing Research Dept.
Cost of Goods Sold	Plant Startup		Manufacturing & Engineering	Operating Co.	Operating Co.: Research Dept. Manufacturing Process Technology Engineering Dept.
Cost of Goods Sold	Process Improvement		Process Research	Operating Co.	Operating Co.: Manufacturing Research Dept. Process Technology Engineering Dept.
	Other		Regulatory Agency Requirements (OSHA, FDA, Environmental, etc.) Patent & Trademark Safety	Operating Co.	Operating Co. (various units) Medical Dept. Patent Dept. Engineering Dept.
	Product/Business Development		Commercial Development	Operating Co.	Operating Co.

Repeat sequence; to *Idea Stage*

*Design Premises Include:

Product Specs.
Raw Material Specs.
Capacity

input than the preceding stages of design. After all, the final designs must all work; there is not the opportunity for trade-off that can occur earlier. Furthermore, the relationships between the final process designer and the other members of the total project team (including manufacturing and construction people) provide opportunity for creativity and innovation in diverse ways.

Zuiderweg (2) characterizes process design work as follows:

> ....experimental work is virtually non-existent. In a way the work is contemplative in that information collected needs to be digested, but on the other hand a great deal of creativity is needed to find optimal solutions to all sorts of problems. [The] people should have a special knack of solving practical operational problems. The courage to stick one's neck out for innovations is another typical requirement. In the field of communications eagerness and perserverance are needed.... [the work] calls for considerable expert support. Among the applied sciences, especially chemical, materials and control engineering are involved: of the general sciences mathematics is probably the most important.

A final stage of process engineering occurs after the plant is in operation. This is the *process improvement* phase, which aids the company in its quest to be the lowest-cost producer of the product(s) involved. Competitive pressures to decrease cost are ever-present, as dictated by the "experience curve" which shows that as the cumulative production of a chemical increases, the deflated average cost of the chemical must decrease (*132*). Process improvement work includes elements of Exploratory Research, Applied Research and Technical Development as well as Engineering. Some organizations define the work as Plant Technical Services, others as Process Technology Services. It involves disciplines that are in common with those of process design, with emphasis more on analysis than synthesis. Process design, process development (R&D related) and process improvement functions are conveniently classified as *process engineering*, as defined in the following section.

B. Process Engineering Defined

Process engineering can be defined broadly as the creation and quantification or analysis of process flow schemes that will form part of an economic, easily operable, and safe plant. Process engineering comprises disciplines or activities which require engineering contributions to process development, process design, and process improvement.

1. **Process Development**

   Process development involves interaction between engineering and research personnel for *conceptual process design* and research-oriented evaluation studies. This could include:

   (a) the evaluation of process for the Research Department
   (b) the evaluation of processes for outside purchase
   (c) help in the development of new processes on bench and pilot plant scales
   (d) the review of existing processes for innovation

2. **Process Design**

   Process design involves assembly of the "process design package," which includes physical property data, flow diagrams, material and evergy balances, equipment performance data, utility schedules, control schemes, and so on. It also involves economic evaluation since its general objective is to arrive at the most economical flow scheme.

   Process design can be broken into general types;

   (a) *Preliminary process design* which are activities and studies directed towards preparation of a captial appropriation request and would include the following activities:
      preparation of flow diagrams
      preparation of material and energy balances
      gathering of physical property data
      feedback to the process design effort
   (b) *Final process design* would involve activities directed towards equipment purchasing and installation and would include:
      preparation of final process and engineering flow diagrams
      equipment performance data
      equipment specifications
      review of detailed piping, mechanical, electrical, and instrumentation drawings

3. **Process Improvement**

   The last category of process engineering could be called *process improvement*. Process improvement activities embody engineering work directed toward improving existing process facilities. The work may be directed toward improved operating strategies and/or modification of physical facilities. Process improvement emphasizes *analysis* whereas process design emphasizes *synthesis*.

C. Purchased Process Technology

The foregoing remarks have implied that propriety process technology is to be developed, and the resulting plant is to be operated efficiently with continuous improvement. Not even the largest companies with extensive resources develop all of their own technology. Thus, process engineering has components of (1) developing design packages for sale or license and (2) analyzing packages of others (in forms ranging from brief disclosures based on patent and published references to detailed scope reports) for processes being considered for purchase or license.

Figure 1, from an excellent article by Spitz (*1*) shows typical steps in evaluating one or more outside processes for possible license. As shown in the figure, preliminary process design has been done by the licensor, and final process

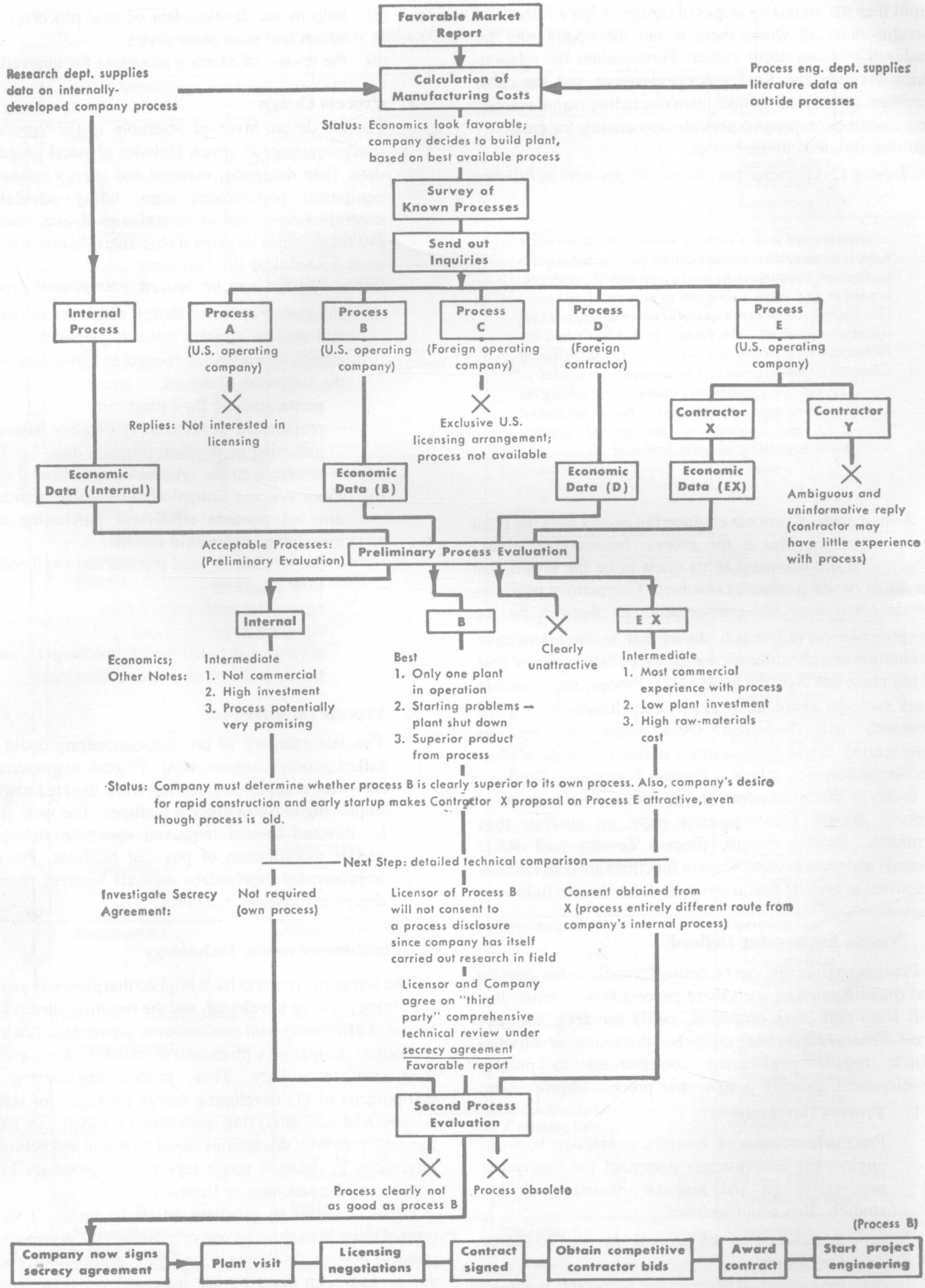

Figure 1. Steps in The Evaluation of Competitive Processes for License (From Spitz, P., *Chem. Eng.* 72 (26) 91 (Dec. 20, 1965)

TABLE 2
QUESTIONNAIRE FOR PURCHASING PROCESS TECHNOLOGY

General

1. Is the process completey defined?
2. How many commercial installations are operating?
3. Can operating installations be visited and examined?
4. If there are no operating installations, does licensor have plans for commericialization?
5. Is the licensor identified with a particular engineering contractor?
6. If so, how firm is the alliance? May we choose another contractor?
7. What is the general reputation of, and our experience with, the contractor allied with the licensor?
8. Is the contractor-licensor team [if any] prone to ''oversell''?
9. Are we prepared to deal with contract problems?
10. Can we evaluate properly any guarantees involved?
11. Is the stream time efficiency based on rational reliability considerations?

Process Development

1. How extensive was the laboratory research?
2. Who did the laboratory work? Their qualifications?
3. May we examine laboratory data to develop our conclusions?
4. How early did Engineering get involved?
5. Was there a bench-scale continuous [if approriate] unit?
6. Was there a semi-works scale unit? With recycle?
7. Were all process steps operated simultaneously with recycle and build-up to equilibrium levels of by-products?
8. May we examine bench-scale and/or pilot plant results?
10. Who did the bench and semi-works scale research? Their qualifications?
11. How complete are the physical property data? Can critically-important data be defined?
12. Have simulation/optimization studies been made? Does the licensor have advanced capability in this area?

Product

1. Are the product specifications realistic? Have they been met in research? Have they been met commercially?
2. Are the specifications complete? Could unexpected contaminants become a problem?
3. Are methods for analyzing product adequate and consistent with those used by customers?
4. Are there problems with storage of product (e.g. stability)?
5. Are there any problems with shipping the product?
6. Do by-products represent problems, such as utilization, disposability, unusual economic leverage?
7. Does the process offer opportunity to up-grade the product [to meet future demands] without excessive cost?
8. How are by-product pollutants to be dealt with?

Raw Material(s)

1. Are specifications on the raw material adequate and realistic?
2. Are methods for analyzing raw material adequate and consistent with those used by suppliers?
3. Have raw material availability and cost been considered on a long-term basis? Long-term commitments?
4. Is raw material available from more than one supplier?
5. If not, does supplier have geographically-separated producing units?
6. Has raw material transportation reliability been considered carefully?
7. Is raw material storage a problem?
8. Will special processing of the feed be required?

The Process

1. Is a detailed flow diagram available?
2. Are material and energy balances available?
3. How much process modeling has been done?
4. What degree of scaleup is involved? Can we cope with the scaleup problem?
5. What degree of ''adjustment'' from existing process background is required (e.g., on throughput).
6. Is all chemistry completely understood?
7. Are flammable, toxic or unstable materials involved?
8. How well have operational safety provisions been developed by the licensor? By the contractor?
9. What special hazards are involved in the process and the process equipment?
10. What have licensor and contractor done to control these hazards and what more needs to be done?
11. How sophisticated are they on design of interlock and alarm systems? Can they handle total control system design?
12. For heat transfer steps, are fouling problems amenable to advance analysis and solution?
13. For reaction steps:
    (a) Is the catalyst properly identified?
    (b) Are catalyst availability and stability well-defined? Has catalyst practice been established?
    (c) Are there alternate catalysts?
    (d) Are there scaleup problems associated with the reactor?
    (e) Are there models for predicting yield and conversion?
    (f) How is the reactor to be started up?
    (g) Is the control system adequate?
    (h) Do materials of construction influence yield and conversion?
14. For the separation system:
    (a) Can contaminants enter the process during the separation steps?
    (b) Are there special separation problems such as ''hidden azeotropes and inconsistent equilibrium data?
    (c) Has the system been demonstrated properly?
    (d) Are there foaming problems?
    (e) Are there control problems?

Economics

1. Are detailed capital cost data available? What is their basis? Do the data represent our equipment erection and general plant constuction practices?
2. Do costs account for possible future price increases?
3. Are detailed manufacturing cost elements available? Do they include sufficient information on maintenance requirements? Can they be interpreted according to company standard cost elements?
4. Is the cost of startup evaluated properly? Are time-manpower provisions by contractor included?
5. Are operating personnel requirements realistic?
6. Is there justification for computer control?
7. Have optimization studies been made?
8. Are all licensing fees and royalties included in the projected costs?
9. Do profitability studies take into account time value of money and future vagaries of selling price?

Miscellaneous

1. Have materials of construction specifications been considered carefully? Test data available?
2. Does equipment fabrication require special shop facilities and expertise?
3. Have procedures for startup, shutdown and decontamination been developed?
4. Have stream and laboratory analytical problems been considered?
5. What hazards are involved?
6. Are licensor and contractor amenable to intensive safety reviews?
7. Have we considered possible future modifications for changed products or capacity increases?
8. Are physical models available for inspection?
9. Is there agreement on specifications/standards to be used?
10. If the proces equipment is to be fabricated in a foreign country, has due consideration been givento shop capabilities, vendor inspection/expenditing, and local design capabilities?

design may also have been done. Accordingly, the purchaser/licensee involvement may range from detailed studies to simple review of final process documents.

The pitfalls of purchasing or licensing outside process technology can be significant. Much will depend on the reputation and general track record of the firm that has developed the technology. Purchases of well-known packages for ammonia, ethylene, styrene, and so on can be done with a high degree of confidence. At the other end of the scale, one can license technology for a process that has never been practiced commercially! Enlightened process engineering advice is clearly a key to analysis of the potential profitability of the newly-developed yet untested process.

A listing of typical questions to be asked by the prospective purchaser/licensee is given in Table 2. Many of the same questions might well be asked within a corporate organization, when internally developed technology is approaching the preliminary or final process design stages.

TABLE 3
TYPICAL PROCESS DESIGN "PACKAGE" COMPONENTS

DESIGN BASIS
MATERIAL & ENERGY BALANCES
FLOW DIAGRAMS
PROCES SPECIFICATIONS ON EQUIPMENT
CONTROL SPECIFICATIONS
UTILITIES SUMMARIES
ENVIRONMENTAL IMPACT DATA
OPERATING PROCEDURES
SAFETY & HAZARD ANALYSIS

D. The Design Package

The classic "process design package" comprises the elements shown in Table 3. It includes one or more flow diagrams, overall and individual mass balances, overall and individual energy balance, specifications for critical equipment items, specifications for control systems, information on utilities, special operating features, and so on. In addition, there are likely to be supporting economic documents. For preliminary design, the package will naturally be sketchy in places. For final design, it supplies enough information to enable the mechanical, civil, electrical, and architectural engineers to take over and put the process into final physical form.

It is of interest to study changes in this package that have occurred during the past 35+ years. In 1942, the pressure of World War II did strange things to the sequence of process design. It was not uncommon for the preliminary step to be all but by-passed. Conceptual designs were scaled to final designs. Empirical models were pushed beyond their limits. There were scaleup fiascos and there were some processes that just couldn't "get off the ground". By and large, however, the plants made the production and the rest is history.

There were some particular marks of the package that should be noted, as shown below:

1942 DESIGNS

Conservative
Approximate
Courageous

The urgency of the times and the general economic conditions just preceding the war were such that *conservative designs* were called for. It was expected by management that equipment would be oversized — that it would be there and available for improved production that would surely be called for. If there was any question about the number of trays required for a distillation column, or the number of bubble caps needed on the tray, or the required column diameter for a certain reflux, the conservative approach was taken. Extra trays were added, allowance was made for additional reflux, and, except for a few cases where this backfired, the idea worked. There were not many times when a process would have to shut down because of undersized separation equipment. The same could be said about reaction equipment; pilot plants were scaled up conservatively; additional reactors were installed in series, the money was spent to make the product on schedule and possible at a reasonable rate of return on investment. So one of the characteristics of process design in 1942 was conservatism. It was affordable, considering the times.

Clearly, the 1942 designs were approximate. Physical property correlations, even for the hydrocarbons, were far from exact. Calculations were all made by slide rule and desk calculator. Engineers then, as now, were in short supply. And, as mentioned earlier, models were likely to be empirical and crudely developed. Thus, a "tight" prediction of operating conditions was often not feasible, and it was common to find instruments completely off-range when production started.

The final item in the 1942 listing deals with the courageous attitude of management as well as the designer. Wartime conditions had their influence, of course, but risks *were* taken and the consequences of failure in a professional sense did not result in vindictive measures. The understood conservatism tempered courage, of course, but it was still there.

Now, let us look at a comparative situation today:

1979 DESIGNS

Tight
More exact
Risk-calculated

Not all designs today have these characteristics. It appears safe to say that today *tight designs* are fairly common. An example might be the competitive turnkey ammonia plants obtainable from several contractors. When handled on a lump-sum contract basis, there is every incentive for a "tight" design to result. This is not to say that management always understands the real meaning of a tight design — unless more throughput capacity ultimately results from expensive debottlenecking!

The exactness, if not the absolute correctness, of designs has certainly improved through the years. High-speed digital computers are used regularly in the design of individual process components as well as full process systems. The influences of transient behavior have been approached more rigorously. The design notebook now contains an extremely large and impressive amount of numerical data.

The last item in the listing shows only that identified tightness and exactness permit a more judicious calculation of risk. Elaboration of this point will be included later under "dependability analysis".

To conclude these remarks on process design history I wish to confront you with a thought which may very well be a fact: *A surprising number of "1942 designs" continue to appear today*. Much of what is termed "modern, systems-oriented design" represents more hope than fact. This can be particularly true in new areas where successive design stages have not evolved a more up-to-date style of design.

II. DATA BASE FOR PROCESS WORK

To the process engineer, "data base" may be synonymous with a source of physical property information. In fact, the engineer uses a wide range of data, some of the "handbook" type but much of which is related to the standards and procedures of the engineering organization. There are, for example, standard equipment sizes, industry codes, metallurgical and corrosion information, site design premises, and so on. During the engineering of a project, countless bits and pieces of information are used and re-used, and a system to manage them for efficient use is mandatory in modern design.

During the past few years, computer technology has advanced to meet the needs of data management. One development is a system by IBM called Information Management System, IMS. This system, which is thought to be typical of those of other vendors, comprises two major components: the data base facility and the data communication facility. The former is in effect a language that allows a programmer to construct and then use a data base. The latter supports remote access of the data base, for storage or retrieval of information; it can be appreciated that for a large engineering project the same data items might be sought and used many times by diverse groups.

The organization and structuring of data systems is a difficult and exacting science. It requires understanding of the likely use of the data as well as the manipulation of the data in the form of correlations. For some applications it is necessary to protect the data in order to maintain its integrity. This developing application to process engineering has not been documented broadly, but there are now a number of operating systems. A description of an earlier system by Phillips Petroleum has been given (*3*). The CHEIS (Chiyoda Engineering Information System) system is thought to be one of the most advanced for chemical engineering needs (*4*). The book by Martin (*5*) provides general approaches to the organization and implementation of data base systems. In its ultimate form, a data base system will interface directly with user programs for analysis and design or, if desired, with an individual seeking discrete information. The application of a system to physical properties, as developed in the following section, should bring the importance of data base systems into sharper focus.

A. Property Data

Types of property data needed for process engineering are listed in Table 4. Ideally, the process engineer could access a data base containing such information and obtain exactly what he needs, the data being of high accuracy. When one reflects on the extreme diversity of chemical systems that might be encountered, he realizes that no system could approach the ideal very closely. Methods for correlating and estimating properties are required, and these often are not well supported. And yet, a reasonable approach to the ideal, for *fluid systems*, is now possible.

TABLE 4
TYPES OF PROPERTY DATA NEEDED FOR PROCESS ENGINEERING

Identification and physical properties
- Molecular weight
- Molecular structure
- Normal boiling point
- Melting point
- Refractive index
- Density
- Vapor pressure
- Critical constants

Thermodynamic properties
- Heat capacity
- Enthalpy
- Heat of vaporization
- Heat of formation
- Free energy
- Entropy
- Phase equilibria

Transport properties
- Viscosity
- Thermal conductivity
- Diffusion coefficient
- Surface tension

Reaction properties
- Chemical equilibria
- Heat of reaction
- Rate constants

A physical property data base should include the following:

1. Authenticated data file
   a. Published information
   b. Proprietary information
2. Unauthenticated data file
   a. Published information
   b. Proprietary information
3. Methods for estimating data
4. Methods for accessing data directly
5. Methods for coupling retrieved data with design models.

B. Data Banks

There are a number of existing data base systems. In a 1978 survey, Rose (*6*) categorized them as follows:

1. Data banks developed by manufacturing or design companies for internal purposes, and later marketed to recover development costs.
2. Data banks developed for marketing purposes.
3. Data banks developed by educational institutions, primarily for teaching purposes.

The results of the Rose survey are shown in Table 5. One must recognize that such surveys do not produce information that remains completely reliable, but at least one point is made clear in the table: an organization does not have to develop its own data bank in order to benefit from a bank availability. All are available, either directly by purchase (including all software) or indirectly by "black box" access through service bureaus.

The FLOWTRAN bank is included in the Table 5 listing and is an example of a widely-used system. It has been described in some detail (*7*, *8*). The data records are stored in the computer as a series of constants for a single chemical (Table 6). For mixtures, or for pure components not covered specifically in the stored files, a computational routine is included for property estimation. This routine requires raw data as shown in Table 7. For liquid-phase activity coefficients of non-ideal mixtures, separate routines are used. The FLOWTRAN system is also typical in that it deals primarily with fluids. With special attention, solid-fluid mixtures in slurry form can be handled.

Output from the FLOWTRAN bank is normally used directly in unit operations models, but it can be prepared separately in printed or graphical formats. There are needs other than for design that are best met on a stand-alone basis, for example the plant technical services engineer seeking density data for instrument calibrations.

There are available other discussions of physical property data systems. Chueh and Stein (*9*) describe a system designed for engineering company use and show typical output data. Yen *et al* (*3*) describe the Lummus/Phillips proprietary system and emphasize problems associated with vapor-liquid equilibrium data correlation. Meadows (*10*) and Norris (*11*) describe a properties program developed under AIChE sponsorship and funded by some 35 industrial and governmental organizations. O'Reilly and Edmonds (*12*) consider the cost of providing a computerized data service, and the savings possible over the manual approach.

Not only can computerized systems be justified on a search/retrieval cost basis, but also on an accuracy basis. Table 8 (*13*) provides a rough guide to the effect of inaccurate physical property values on size and cost of equipment. The percent errors shown are typical for the properties involved. The effects of these errors are estimated on the basis of normal application and standard design methods. Thus, there are incentives both in engineer productivity and in capital cost that aid the justification of data base systems.

C. Current Work in Data Development

A big problem with physical property data base systems is that they must cover large gaps between and beyond measured, authenticated property values. Chemical companies which process a wide range of raw materials and intermediates are particularly concerned with this problem. Much aid has been provided by research sponsored by the National Bureau of Standards, American Petroleum Institute, Office of Scientific Reference Data, and other organizations. A private research institute, Fluid Properties Research, Inc. (FPRI) is funded by a number of companies, but results are confidential (*14*). In 1978 a new consortium, Design Institute for Physical Property Data (DIPPR), was formed under the aegis of AIChE: this industry-sponsored consortium will organize and evaluate existing data as well as fund measurement of new data. Results will be publicly available. The initial contract, covering an analysis of existing information, will be handled by Pennsylvania State University.

A particular data base problem rests with the behavior of non-ideal systems so far as their fluid phase equilibria are concerned. A massive effort is underway at several institutions to organize what data have been reported and then make available more reliable information in the form of measured or correlated properties. These phase equilibria affect the separation factor included in Table 8; the effect of error at low values of the factor is striking.

In the United States, the outstanding VLE compilation effort is at the Thermodynamics Laboratory of Washington University in St. Louis. Over 24,000 literature documents have been retrieved; careful evaluations of properties of 108 pure compounds (mostly C_3 through C_6 hydrocarbons) have been made; consistency tests have been completed in many VLE studies; and significant progress has been made on methods for correlating mixture properties (*15*).

Also in the VLE area, improved models for estimating liquid-phase activity coefficients, when little or no experimental data exist, are being eveloped. Several years ago regular solution theory (*134*) was thought capable of providing a basis for such *a priori* estimation of the coefficients.

Table 5

DATA BANKS FOR PHYSICAL PROPERTIES

(from survey by Rose (6)

Survey Date: March 1978

Organisation	Bank Name	No. of Chem. Compounds & Type(1)	Availability(2)	Number of Properties	"Flash" Calculation	Provisional Extension of Components List	Remarks
Category 1:							
I.C.I. Mond Division	DATABANK	500 (c)	Purchase of "Software" but no Data	40 + 14 VLE	YES	read in own data	Extensive data bank; software only can be bought.
Monsanto	FLOWTRAN	180 (m)	Purchase	10 + 4 VLE	YES	use special file	Must be used with FLOWTRAN. Appears to be a minimal number of properties, the emphasis being on FLOWTRAN and not data.
Solvay	CBM	200 (m)	Purchase	29 + 2 VLE	YES	special code numbers	A bank developed for internal use, and later decided to market
DSM	TISDATA	120 (h)	Purchase and Bureau	25 + 4 VLE	YES	read-in own data	Developed for own use, now marketed, predominantly hydrocarbon.
Uhde	Uhde Stoffdaten Compiler	"Several thousand" (m)	Purchase	17 + 3 VLE	YES	Program generates from structure	Extensive industrial bank

TABLE 5: DATA BANKS FOR PHYSICAL PROPERTIES (cont'd.)

Organisation	Bank Name	No. of Chem. Compounds & Type(1)	Availability(2)	Number of Properties	"Flash" Calculation	Provisional Extension of Components List	Remarks
Category 2a:							
DSM (see also category 1)	TISDATA	120 (h)	Purchase and Bureau	25 + 4 VLE	YES	read-in own data	Marketed through DSM-owned Computer Bureau.
Inst. Chem. Engineers	PPDS	412 (m)	Purchase, Bureau and Leasing	32 + 2 VLE	Next Year	"input own data"	A bank created to be a service to outside users.
DECHEMA	DSD	410	Purchase from Uhde Bureau from DECHEMA	24 + 6 VLE	YES	can be generated	Bank developed for outside users. Extensive.
CHEMSHARE (Europ. representative Maute & Becker)	CHEMTRAN	850	Bureau	8 + 0 VLE	YES	user can enter	Minimum data to enable property generation for calculation.
LASSC Liège University	EPIC	250 (m)	Purchase and Bureau	16 + 6 VLE	YES	extend bank	University bank aimed at industrial use.

TABLE 5: DATA BANKS FOR PHYSICAL PROPERTIES (con't.)

Organisation	Bank Name	No. of Chem. Compounds & Type (1)	Availability (2)	Number of Properties	"Flash" Calculation	Provisional Extension of Components List	Remarks
Category 2b:							
NPL	Org. Systems VP & VLE	500	by post only	1 + 5 VLE	YES	- - - -	Bank used by CAD Centre and PPDS. Excellent range of VLE correlations
University of Sussex	Computer Analysed Thermo-Chem. Data	4000	Purchase	2 + 0 VLE	---	- - - -	Only Ht formation and latent heat of organic and organo-metallic compounds.
NPL / Association Thermodata	MTDATA (GEMT)	2000	Bureau and Leasing	5 + 0 VLE	---	- - - -	Specific bank to therm. changes in inorganic solution reactions.
Dortmund University	DDB		Bureau and Leasing	0 + 5 VLE	YES	uses UNIFAC	An excellent VLE bank.
TRC/API	TRC Data Bank	250 (m)	Bureau planned	12 + 0 VLE	NO	- - - -	Primarily for recovery of fluid thermodynamic data.
NEL	NEL-APPES	200 (m)	Purchase - Bureau	17 + 0 VLE	NO	- - - -	Emphasis on comparison of predictive methods (160 methods available). Not for direct use with engineering programs.
Tokyo University	EROICA	7500	Purchase - Bureau	11 + 0 VLE	NO	- - - -	Emphasis on complete coverage of a limited range of properties.
Purdue University	CINDAS	14000 (m)	Purchase and Bureau	7 + 0 VLE	NO	- - - -	Emphasis on complete coverage of a limited range of properties.

TABLE 5: DATA BANKS FOR PHYSICAL PROPERTIES (cont'd)

Organisation	Bank Name	No. of Chem. Compounds & Type (1)	Availability (2)	Number of Properties	"Flash" Calculation	Provisional Extension of Components List	Remarks
Category 3: Edinburgh University	---	50 (m)	Teaching	15 + 1 VLE	YES	extend bank	Clearly a bank intended for internal teaching use.
Manchester University	Physical Property Data System	80 (h)	Teaching	18 + 0 VLE	NO	- - - - -	Clearly a bank intended for internal teaching use.
Milan Polytechnic	PHYSCO	60 (h)	Teaching	10 + 6 VLE	NO	extend bank	Emphasis on hydrocarbon mixture data and comparison of different methods.
EURECHA (European Universities)	CHEMCO	54 (m)	Teaching	16 + 1 VLE	YES	read-in own data	Bank intended for teaching use.
Washington University	CHESS	80 (h)	Teaching	- - -	YES	- - -	For use with the CHESS Flowsheet Program.

KEY TO TABLE :

1. c = general "Chemical" compounds
   h = mainly hydrocarbon compounds
   m = both (c + h)
2. Bureau = access through Computer Bureau
3. i.e. 10 + 3 VLE means 10 properties for 1-phase-mixture and 3 methods for VLE (Wilson and Redlich-Kwong are the most common)