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# THE NATURE AND ROLE OF PROCESS SYSTEMS ENGINEERING

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Abstract. In this article the author is going to attempt to establish Process Systems Engineering as an important core field in Chemical Engineering. Therefore, the definition of Process Systems Engineering, its necessity in the field of Chemical Engineering, its philosophical backbone and an opinion on the general structure of Process Systems Engineering are given first. Later, the important roles which Process Systems Engineering have played in the past and will have to play in the future are mentioned with concrete examples of research done in the author's laboratory. The need for continuous research and developement in this field is stressed in conclusion.

## THE DEFINITION OF PROCESS SYSTEMS ENGINEERING

The meaning and contents of any technical terminology may change with the times and according to the state of the field in which the term is used. At this point in time, the definition of "PROCESS SYSTEMS ENGINEERING" may most adequately be given by an explanation of "Engineering for Process Systems" or "Systems Engineering for Processes".

"SYSTEMS ENGINEERING" is defined as an engineering field and methodology for making engineering decisions in a system which is composed of many sub-systems or parts and has to satisfy and achieve any given set of conditions and objectives. It can be easily recognized from the above definition that any of the unit operations and production processes related to "Chemical Engineering" are considered to form a system. Systems Engineering has no specific object in itself, but rather is concerned with general methodologies for engineering decision-making, for example, for planning, design, management, control and so on. On the other hand, Process Systems Engineering has specific objects related to Chemical Engineering, that is, unit operations, chemical processes, chemical industries etc. Because much analytical information to express the characteristics of these objects has thus far been accumulated, it may be essentially important in Process Systems Engineering to effectively combine general methodologies and the characteristics of the individual objects.

In short, Process Systems Engineering can be defined as follows: "It is an academic and technological field related to methodologies for chemical engineering decisions. Such methodologies should be responsible for indicating (i) how to plan, (ii) how to design, (iii) how to operate, and (iv) how to control any kind of unit operation, chemical and other production processes and chemical industries themselves".

## CHEMICAL ENGINEERING AND PROCESS SYSTEMS ENGINEERING

Chemical processes which produce a great number of chemical products are composed of a rather small number of unit operations including chemical reactors compared with the number of processes. The need for an academic field of Chemical Engineering arose due to the fact that all chemical processes must be reasonably constructed according to the principles of design for unit operations. In other words, if all chemical processes are analyzed functionally, it may be recognized that every chemical process can be regarded as a combined system of unit operations, as shown by the axes from OA to OB in Fig. 1.

In order to improve unit operations and develop a new unit operation, it is important to quantitatively understand the fundamental phenomena which are generated in unit operations. Based on this concept, so-called "Chemical Engineering Sciences", such as Transport Phenomena, Fluid Dynamics, Thermodynamics, and Chemical Reaction Kinetics and others have been emphasized since around 1950. In other words, every unit operation can be identified as a combined system of fundamental phenomena , as shown by the axes from OB to OC in Fig. 1.

A very natural question arises here : "Can we make any reasonable engineering decisions about unit operations and chemical processes by only having enough technical knowledge of fundamental phenomena ?" More precise and deeper analysis of phenomena are always important from the analytical point of view in engineering fields. However, if the final goal of chemical engineering can be regarded as making decisions on the design and operation of chemical processes and unit operations, methodologies are required for making such decisions. In this case, analytical information of fundamental phenomena may be useful to make decisions on unit operations, and the information of unit operations on chemical processes.

Process Systems Engineering should be consist of a methodology aimed at fulfilling the above requirement. Describing Fig. 1, the axis OX of Process Systems Engineering rotates through all of the quadrants in the figure, and should play the important role of mediating between the axes from OC to OB and OB to OA.

As was mentioned above, Chemical Engineering originated from the point of view of the design of unit operations, but its final objective must be the reasonable, effective design and operation of chemical processes. Here, one thing should be noticed. All chemical processes should not exist independent of their surroundings. Rather, they must be reasonable and effective from the point of view of the larger system which includes each chemical process as a sub-system. In Fig. 1, all chemical processes expressed on axis OA should be responsible for the larger systems explained on axis OD. In other words, Process Systems Engineering should also contribute to planning chemical complexes, to solving environmental and energy problems at both the regional and national levels, and to making engineering decisions on other global problems.

In the above description, functional matters were mainly covered, but these functions of unit operations and chemical processes are performed in many hard systems, such as unit apparatuses, pipe-lines and chemical plants. Therefore, a discussion similar to that above may be possible for hard systems, but only functional and soft systems will be discussed in this paper.

## ANALYSIS AND SYNTHESIS

It may be clear from the previous discussions that Process Systems Engineering should contribute to synthesizing any size of system related to chemical engineering. In this paper, the word of "Synthesis" is commonly used to mean planning, design, operation and control which are kinds of chemical engineering decisions.

The direction of Synthesis is the opposite of Analysis in Fig. 1, and analytical information is required to synthesize a system in which the information exists. Since the relationship of analysis and synthesis is the inputs and outpus of a system, it may be meaningful for clarify the role of Process Systems Engineering by taking notice of the characteristics of Analysis and Synthesis.

A definition of "Analysis" may be given as, dividing a system into a definite number of subsystems and making clear the characteristics of each subsystem. In order to under-

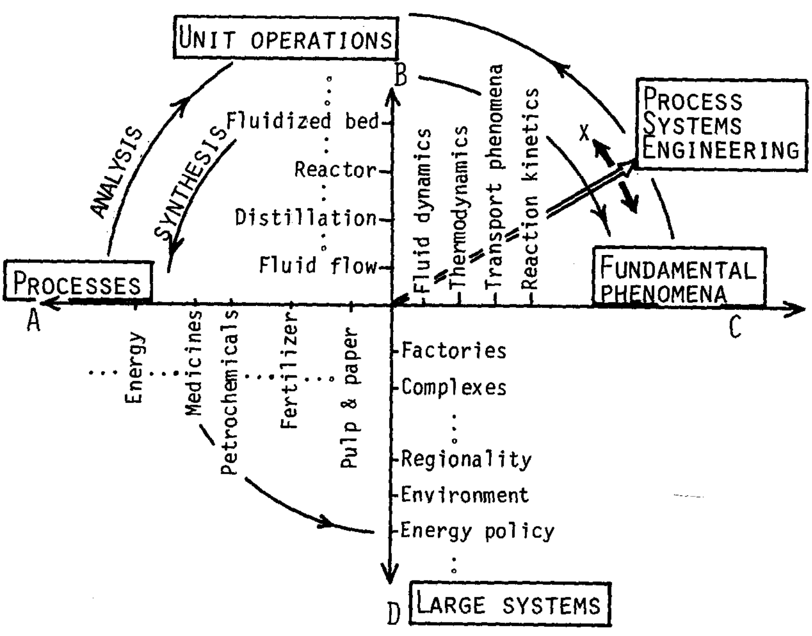


Fig. 1. Process Systems Engineering and Chemical Engineering

take such clarification, the subsystem should be divided again into smaller parts, and the characteristics of each part should become clear. However, proceeding according to the above concept, one may be faced with unknown or uncertain phenomena despite the fact that the academic field of chemical engineering analysis has been developing for several decades. Many chemical engineers are doing important analytical work in an effort to make improvements in this situation. Even if one were able to obtain perfect analytical information on a system, information of the infinite number of infinitesimal elements is really necessary to explain the characteristics of the system, not to mention the infinite time that would be required to obtaine such information. In short, perfect analytical information cannot be obtained in a definite time, and so any analytical information which is necessary to synthesize a system necessarily includes some uncertainties.

On the other hand, when going to synthesize a system, conditions related to the inputs, outputs and objectives of the system to be synthesized should be given prior to synthesizing. Generally speaking, the system to be synthesized is a sub-system of a larger system which includes the system to be synthesized. The input- and output- conditions as well as the objectives of the system to be synthesized should be given from the point of view of the larger system. Proceeding from the above concept, when attempting to obtain perfect information on the input- and output- conditions and the objectives of a system to be synthesized, all cause and effect relationships in the infinite universe should be made clear. However, recognizing the uncertatinties of the conditions and objectives, this is of course impossible.

Fig. 2 schematically shows the concepts for Analysis and Synthesis mentioned above. The following three subjects arise as important practical problems to solve in the field of chemical engineering:

(i) How precise the analytical information needs to be, and how much is enough to synthesize a process system ?

(ii) How large of a system is necessary to determine the input- and output- conditions and the objectives for a process system to be synthesized ?

(iii) How fast can engineering decision problems be solved ?

The solution of these three basic practical problems will be critical in the development of Process Systems Engineering.

## A BRIEF HISTORY OF PROCESS SYSTEMS ENGINEERING

Many mathematical optimization techniques, for example Dynamic Programming, the Maximum Principle and others, have been rapidly developed since around 1950. The academic field of Process Systems Engineering was born for the purpose of applying these mathematical theories to the optimal design of unit operations. The importance of the concept of the economical design of unit operations has been advanced in the field of chemical engineering for a long time, but methods for this purpose were mainly empirical and numerical for rather simple unit operations. Since around 1950, the economic design and operation of rather complex unit operations have come to be easily accomplished by introducing mathematical optimization theories into the unit operations design method.

As described in the previous section, the optimality of a unit operation should be evaluated from the point of view of a chemical process which includes the unit operation Also, the goal of chemical engineering itself should be not only the design of unit operations but the design and operation of chemical processes as well. Therefore, Process Systems Engineering, which was born for the purpose of the optimal design of unit operations, has developed and expanded into the direction of the design and operation of chemical processes. As a process system to be synthesized becomes larger and more complex, the objectives for the process system expands from one to many. It might be enough from the practical engineering point of view to design a simple unit operation, for example a heat exchanger only under an economical evaluation, but it may be necessary for the design and operation of chemical processes to make an engineering decision under the condition of multi-objectives. Economical conditions, environmental assessment, safety, operability, flexibility for change of raw and energy

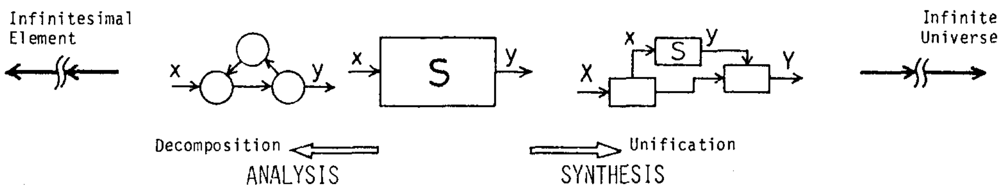


Fig. 2. Analysis and Synthesis

materials etc. are some concrete examples of these multi-objectives.

Many of the objectives mentioned above are closely related to process operation rather than design, and it may be possible to judge whether the design of the process system is good or not only after practically operation of the process system designed. Both Chemical Engineering and Process Systems Engineering have been generated for the purpose of the design of unit operations. However, now, design taking into consideration the operation or integration of design with operation should be considered in the field of process systems engineering. In order to achieve the integration of design and operation, it is necessary first to establish methodologies for decision making for process operation which includes process control system design. Then, the operational information obtained by this methodology should be used in the design stage of the process using the principle of feedback. In the future, a coupling and integrated method for decision making for design and operation may be developed.

As mentioned above, the content of Process Systems Engineering has been expanded from the design of unit operations to the design of chemical processes and the planning of large process systems, as well as from design problems to operation or manipulation problems, and in addition to having gone from single objective optimization to multi-objective optimization. It should be noticed that this expansion has been made feasible due to rapid development of electronic computers. The fact that terminologies, such as Computer-Aided Design, Computer-Aided Operation, and Computer-Aided Management are widely used in the field of Process Systems Engineering shows the importance of computer use and computer technology in the development of Process Systems Engineering. However, it should be emphasized that "Process Systems Engineering" is not identical to "Computer Application in Chemical Engineering" but it has a more philosophical and methodological backbone. Each core field of chemical engineering, such as Transport Phenomena, Chemical Engineering Thermodynamics, Chemical Reaction Engineering, Engineering, Unit operations, and Process Control has a philosophical and methodological backbone as well as its own general structure. Therefore, the general structure of Process Systems Engineering must then be shown to be one of the core fields of Chemical Engineeing.

## THE GENERAL STRUCTURE OF PROCESS SYSTEMS ENGINEERING

Whenever one is going to synthesize a process systm, one need to have the analytical information, conditions and objectives which are related to the system. Fig. 3 shows a general structure for a Process Systems Engineering methodology. In order to explain the content of Process Systems Engineering, several ideas can be used to divide the content into subsystems. For example, the following kinds of classification are possible:

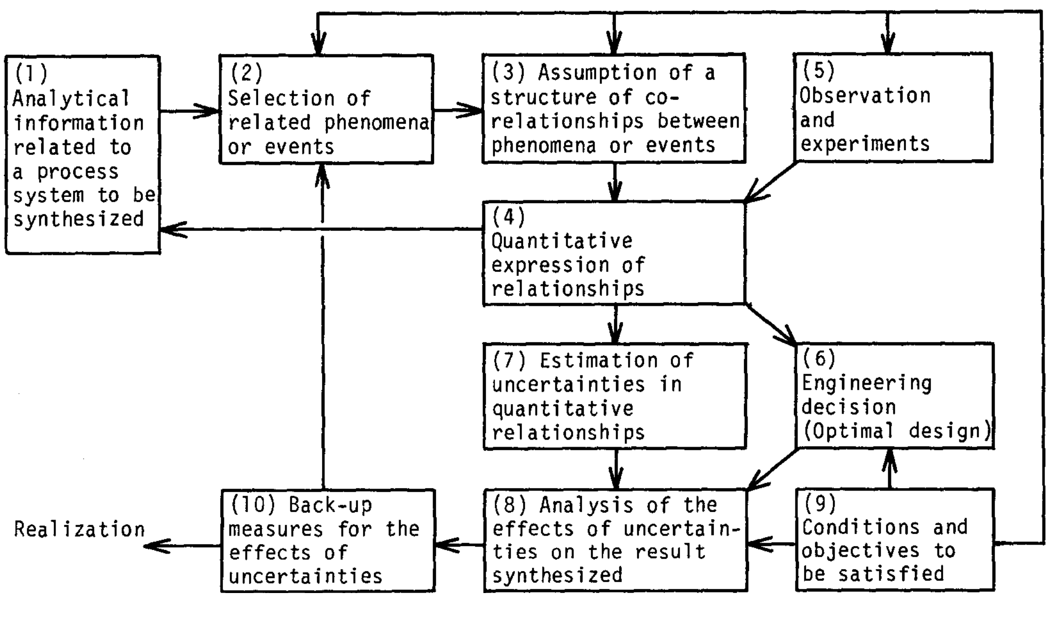


Fig. 3. A general structure of process systems engineering

(A)

- Modelling (Identification)
  - Statics
  - Dynamics
- Synthesis
- Analysis of solution
- Evaluation
- Decision making
- ⋮

(B)

- Data processing
- Simulation
- Optimization
- Control & systems theories
- Scheduling
- ⋮

(C)

- Unit operations
- Chemical processes
- Chemical factory
- Chemical industry
- ⋮

(D)

- Planning
- Development
- Design
- Construction
- Operation
- Management
- Maintenance
- ⋮

The classification shown in Fig. 3 is nearest to the classification of (A), but the following points are emphasized in the classification: There is necessity to (i) clarify the relationship between each work included in the Procees Systems Engineering Approach (the Contradiction of Separable Hypothesis for Modelling and Synthesis), (ii) consider the effect of uncertainties on the result of synthesis (True Engineering with the Consideration of Unavoidable Uncertainties), and (iii) grasp the structure of Process Systems Engineering as a common methodology for any kind and size of process systems related to chemical engineering (from Fundamental Phenomena to Industrial Structure).

Some important aspects of Fig. 3 are as follows:

(2): Difficulty of Selection of Related Phenomena

Whenever a process system is to be synthesized, information on the phenomena or events being carried out inside the system is needed. As described in Section 3 the number of types of analytical information related to a process system is nearly equal to infinity. From the prctical point of view, it may not be effective to use totally precise information to synthesize a process system. This is because a certain allowable range for each condition or objective to be satisfied in the synthesized systems generally exists. Also, all analytical information related to a system does not always have the same degree of effect on the conditions and objectives to be satisfied and the values of decision variables of the synthesized system. Up to now, there has been no general method for determining, prior to synthesizing, how many types and what kind of analytical information should be used to synthesize a process system.

(3), (4) and (5):Basic Questions in System Identification

A great number of papers have been published and practical applications made on methods to quantitatively identify the relationships of phenomena or events related to a system to be synthesized under the conditions of a given structure of relationships, as well as on data from observations and experiments. Concerning the determination of the structure of the relationships between phenomena or events, however, empirical and intuitive determinations have been widely done based on many results obtained by analytical research. This stage of determining a structure of relationships is closely related to the selection of phenomena or events stage (2). However, it should be noticed that the structure of the relationships cannot be uniquely determined only from the fact that an assumed structure can explain a definite number of observed or experimental data. Generally speaking, plural structures which can explain the same data can be found for a system, and the optimal decisions obtained from these plural structures are differant from each other. One wonders if its possible to develop a systematic method of determining an appropriate system structure for a given condition or objective of a system to be synthesized ?

(6), (7) and (8) : Uncertainties and Deterministic Engineering Decision

The uncertainty of information in a process system is often expressed by a statistical and stochastic quantity, but engineering decision making should be given deterministically. Any kind of process systems engineering procedure can be regarded as a kind of information processing procedure. Therefore, when analytical information uncertainties are given by statistical quantities, it becomes a practical problem of determining at what stage of information processing a statistical quantity should be transferred to a deterministic quantity in order to make a decision. Every chemical process has the characteristic of "One of a kind". Thus, a quantity of uncertainty of analytical information for a process system is usually given by a deterministic quantity in a movable range in the field of Process Systems Engineering, especially in design problems. Therefore, deterministic procedures for making optimal decisions are usually taken by using the average values to express the relationships. Process Systems Engineering has been developed focusing on this methodology for making deterministic optimal decisions, and many papers have been published for unit operations, chemical processes and a few larger systems.

As described in the previous section the development of a systematic method for solving operational problems in unit operations and chemical processes related to multi-objective problems.is now required. In such operational problems, decision making based on statistical or stochastic information processing may be useful and practical. The application of the stochastic control theory to operational problems for chemical processes should be actively considered.

(10) : Back-up for Uncertainties

Generally speaking, with a back-up at the design stage and one at the operational stage, it may be possible to eliminate the the undesirable effect of uncertainties included in a process system. A design margin and the establishment of a process control system serve as back-up for the undesirable effects of uncertainties included in unit operation. So far, design and operation or manipulation have been decided and performed separately. The unification of design and operation should be considered, including the optimum planning and allocation of back-up systems for uncertainties.

Along with the general methodology described above, the important roles which Process Systems Engineering has played and has to play in the feture are mentioned in the following sections. Reference is made to the work done in our laboratory.

## PROCESS SYSTEMS ENGINEERING FOR UNIT OPERATIONS

As far as can be determined, the terminology of Process Systems Engineering appeared as the title of CEP Symp. Series No. 46, Vol. 59 (1963) for the first time. The major contents in this issue was on the dynamics and control of several unit operations, and did not include the concept of optimal decisions. At that time, research on the identification and optimum operational profile of unit operations was carried out at the initial stage of Process Systems Engineering. Fig. 4 shows the transition to design of a unit operation from the general structure of Fig. 3. A procedure for identification may be given by blocks (2), (3), (4) and (5). In parameter identification shown in block (4), the gradient methods have been effectively used in chemical and biochemical reactors (Takamatsu and co-workers, 1965, 1969b, 1970b, 1970c). As is well known, flow pattern or fluid mixing in a unit operation has a strong effect on its model structure. The obtained optimal policy depends on the kind of model structure used to solve the optimization problem, especially where a nonlinear reaction is performed in the unit operation. Much research on model structure caused by the flow pattern in a stirred tank, sedimentation vessel and also column operation has been done with experimental confirmations (Takamatsu and co-workers, 1965c, 1966b,1967a, 1967b, 1967c, 1967d, 1967g, 1967h, 1968a).

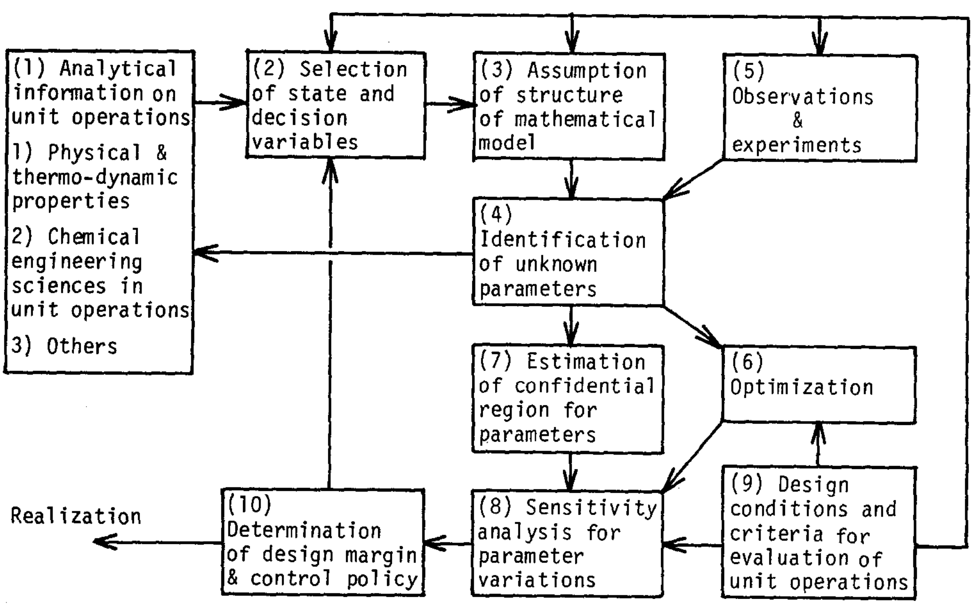


Fig. 4. Process systems engineering for unit operations

Research on obtaining the optimum operating temperature profile of a chemical reactor has been carried out for several types of chemical reactions by using mathematical optimization theories, such as the maximum principle and the maximum gradient method. Also, the effect of the flow pattern on the optimum temperature profile has been considered for batch and continuous chemical reactors(Takamatsu and co-workers, 1965a, 1967e, 1967f, 1967i, 1969d, 1973b). A biochemical reaction process is one of the most complex rate processes, and the determination of (2) and (3) in Fig. 4 is very difficult. Therefore, many problems remain to be solved on the identification of structure and on the optimal operational mode (batch, semi-batch, continuous) for these biochemical processes (Ohno, Nakanishi and Takamatsu, 1978a, 1978b; Takamatsu and co-workers, 1972a, 1973a, 1975a, 1976, 1977a, 1977b, 1978a, 1978b, 1979h, 1980a).

In research on optimization for unit operations shown by block (6) in Fig. 4, mathematical optimization theories studied by theorists have been effectively applied. Also, some new methods suitable for solving optimization problems for unit operations have been developed. For example, a new optimization method under the condition of state-constraint, and a new computational method for obtaining the optimal discrete control and improvements of the gradient method etc have been reported on (Oi, Sayama and Takamatsu, 1972, 1973; Takamatsu and co-workers, 1969b, 1969c, 1978a, 1978b, 1978c).

As shown by blocks (7) and (8) in Fig. 4, the consideration of the effects of uncertainties of parameters in mathematical model and of the conditions of input into a unit operation on the values of decision variables, the output conditions to be satisfied and an objective function are important from the practical engineering point of view. For this purpose, consideration of the concept of sensitivity analysis has been effectively used (Takamasu and co-workers, 1965d, 1966a, 1968b, 1969a). It should be particularly noticed that a method for synthesizing a back-up system for uncertainty, that is, addition of design margin or the establishment of process control, has been given by an application of sensitivity analysis (Takamatsu and co-workers, 1968c, 1970a, 1971b, 1973c). So far, not much consideration has been given to the effect of the deviation of optimum decision variables on the output value to be fixed or the value of the objective function. However, this problem may be important in considering how sensitive the change of the optimally determined manipulating variable is to the deviation of the controlled variable to be fixed and to the value of objective function. This is because the selection of manipulating variables in a process control system may be made feasible based on this consideration (Takamatsu and co-eorkers, 1966a)

As described above, a systematic approach to the optimal design of unit operations has been, for the most part, established by using mathematical techniques and computer to obtain the numerical solution, but there still are many problems to be solved. The fact that a model of the structure of a stirred tank depends strongly on the flow and mixing pattern in the tank.has been mentioned but it may be possible to make many mathematical models based on precise flow patterns and several methods of expression for each flow pattern. The precision and structure of a m thematical model affects every engineering decision synthesized by using the model. A mathematical model may be needed to satisfy an allowable range of deviation of given conditions to be fixed and of the objectives of the process system synthesized by using the model. At the present time, only the concept that the more precise the model is, the better the synthesized result is, is used to determine stages (2) and (3) in Fig. 4. However, using too precise of a model is not necessary and infact is often harmful .

Up to this time , much research on identification has been done under the given condition of observed and experimental data. However, the optimum plan to obtain enough necessary experimental data should be established based on an idea that the effects of parameter deviations identified by using experimental data on the performance of a system synthesized by using the mathematical model are different from each other (Takamatsu and co-workers, 1971a).

As seen in CEP Symp. Series No. 46, many research on the Process Dynamics of unit operations, especially on distillation columns, was carried out at the initial stage of Process Systems (Mizushina and Takamatsu, 1959a, 1959b; Nakanishi and Takamatsu, 1969; Takamatsu and co-workers, 1961, 1962, 1963a, 1963b, 1963c, 1963d, 1964a, 1964b, 1965b). This research might be meaningful to obtain analytical information on the dynamic characteristics of each unit operation. However, it is still not clear what kind of dynamics and how precise of a dynamic model are necessary and sufficient to solve a unit operation problem, especially one related to its control system design.

During the development of Process Systems Engineering for unit operations mentioned above, many computer programs for unit operations were published and used in practice. For example, there are more than 50 simulation programs for a distillation column, but there isn't enogh information on what program is how useful to solve what kind of problem. Also, in our laboratory a method for the simulation of a distillation column has been developed by using an iterative procedure with a physical meaning which might be effective to solve a non-ideal distillation system (Naka, Araki and Takamatsu 1977), but there has been no confirmation to date that this is the best method. Up to this time, many programs have been mainly concerned with unit operations which deal with fluids, but there have been very few concerned with unit operations for solids and powders.

Summerizing Process Systems Engineering for unit operations, the followings may be concluded:
(i) The methods for making engineering decisions for unit operations, including back-up systems for uncertainties, seem to have been, for the most part, established under the conditions of a given model structure and observed or measured data;
(ii) Process Systems Engineering has not yet offered any effective methods for determining model structure or for planning what kinds of observed data are necessary and sufficient to identify a model which will be used to synthesize a process system;
(iii) Although the methodologies for design have been well studied, the characteristics of the optimally synthesized results have not yet been summerized conveniently so as to be used easily and practically without complex calculations by computers;
(iv) It may be necessary to classify the characteristics of many simulation programs and to make clear the effectiveness of each program based on the purpose for which it is used, and finally
(v) Simulation programs for dealing with solids and powders, for example, drying, mechanical separation and so on, should be developed.

## PROCESS SYSTEMS ENGINEERING FOR CHEMICAL PROCESSES

As described in the previous section, optimal engineering decisions for unit operations should achieve the optimum synthesis for a process system. Therefore, Process Systems Engineering has been directed toward synthesizing a chemical process included unit operations. Generally speaking, a chemical process is more complex than a unit operation, and the number of state- and decision- variables in a chemical process is surely more than that in a unit operation. The essential point for synthesis may be the same in both unit operations and chemical processes as shown by Fig. 3. However, a chemical process has the characteristics of a network combination of many unit operations. Therefore, a chemical process is desirable for effective synthesis using the above characteristics.

One of the mathematical optimizing techniques developed to solve a large, complex problem is the so-called "multi-level technique". This technique can be effectively used to solve any synthesis problem for a chemical process in which the structure of a combination of unit operations is given. For example, an optimum sizing problem for each unit operation in a water treatment process which has a rather simple combination structure has been effectively solved by this multi-level technique (Naito and Takamatsu, 1969a,1972; Takamatsu and co-wokers, 1972b). This technique has also been applied to the problem of the optimum sizing of a heat exchanger network with a given structure (Takamatsu and co-workers, 1970a,1976b).

In order to optimally synthesize the network of a chemical process by using usual maethematical optimization techniques, it may be necessary to construct a unified network which includes all thinkable networks in order to give some desired design conditions and objectives, as well as to solve the problem by a suitable optimizing technique, for example the multi-level technique. Based on this idea, the optimal structure of a chemical process is given as the result of optimizing calculations (Takamatsu and co-wakers, 1976a,b).

A problem of the synthesis of a large and complex chemical process may consist of many algebraic and differential equations including many state and decision variables, that have to be solved. The local coordinate system in a set of so many equations has to be found systematically because the number of variables is more than that of the equations found in usual synthesis problems. In order to solve this problem, an application of graph theories has been studied and an effective calculation method to clarify the characteristics of the solution-space of a set of equations has been developed (Takamatsu and co-worker, 1976c). For example, minimizing the number of iterative calculations and tearing points can be systematically achieved by this method. It may be useful in developing a simulation program for a chemical process if this method is applied to making clear the relationships between the inputs and the outputs of each unit operation in a chemical process. This is because a matching procedure for the inputs into a unit operation and the outputs from another unit operation is required for a computer simulation procedure called "the modular approch" (Takamatsu and co-workers, 1976d). When this method is directly applied to a total process including many units, it corresponds to a simulation procedure called "equation-based approach".

As described previously, if the relationships between any specified inputs and outputs for each unit operation in a chemical process can be systematically obtained by the above structural analysis for a set of equations, many process structures are generated in combination by connecting the input and output terminals of each unit operation under the condition of a given kind and number of unit operations. This idea has been effectively used to develop a method for designing a multi-effect evaporator process and a multi-distillation columns process for multi-components (Takamatsu and co-workers, 1975b,1978e). In these cases, some heuristic rules should be effectively introduced to simplify the combination problem. Since a heuristic rule should be based on some individual characteristics of an object to be synthesized, the following problems many naturally arise: 1) how to develop a method in which some heuristic rules may be easily introducible; 2) what kind of heuristic rules should be effectively extracted to combine with a general methodology, and the optimal combination of a kind of general methdology and its set of heuristic rules.

Here, let us consider a general structure of Process System Engineering for chemical processes. Fig. 5 shows a general methodology for making engineering decisions on design problems in a chemical process. It seems that this figure is also meaningful for solving operational problems in a chemical process. A general methodology for solving operational problems will be given later and separately from static design problems.

Adding a short description about some blocks in Fig. 5, it should be noticed first that all stages in Fig. 5 may be performed in a direct computer-aided manner rather than by solving a mathematical problem. In block (3) the method used to solve a synthesis problem in a chemical process in the modular and the equation-based approaches are included. One of the most difficult problems may be in block (4) which calls for the optimal allocation of the degrees of usage of a method using a general method and of a method using some heuristic rules based on the individual characteristics of the chemical process.

It has been mentioned previously that the multi-level technique could be effectively used to solve the problem of the synthesis of a chemical process. An interesting method called "the maximum sensitive method" has been developed to solve an optimal sizing problem for unit operations in a chemical process under the condition of given kinds of unit operations. The idea in this method is based on the following natural fact . That is, when one installs only one very small element of unit operation in order to make the greatest change from the given input conditions to the desired output conditions in a chemical process, the best allocation of the small element may be performed at the location where the maximum sensitivity to change from the inputs to the outputs conditions is shown. The above idea leads to the fact that when the optimal sizing problem is solved, each value of sensitivity in the installation of a small element into every unit operation with the given output value is the same as every other (Takamatsu and coworkers, 1976a,b).

As mentioned previously in the section on GENERAL STRUCTURE, the objective of synthesizing ought to be changed from single to multiple as the boundary of a process system to be synthesized expands from unit operations to chemical processes. At the present time, dealing with a design procedure for a chemical process as a multi-objective optimizing problem is not yet popular in the field of Process Systems. However, an interactive method for multi-objective linear programming has just been developed and applied to the solution of an extension problem concerned with the amount of dealing rate in a chemical process (Takamatsu and cowarkers, 1981g).

It may be meaningful and valuable to study the methods for directly obtaining the optimum decision variables by solving multi-objective problems. However, it seems to be important that a reasonable method for solving the problem of synthesis in a chemical process with an individual objective, for example

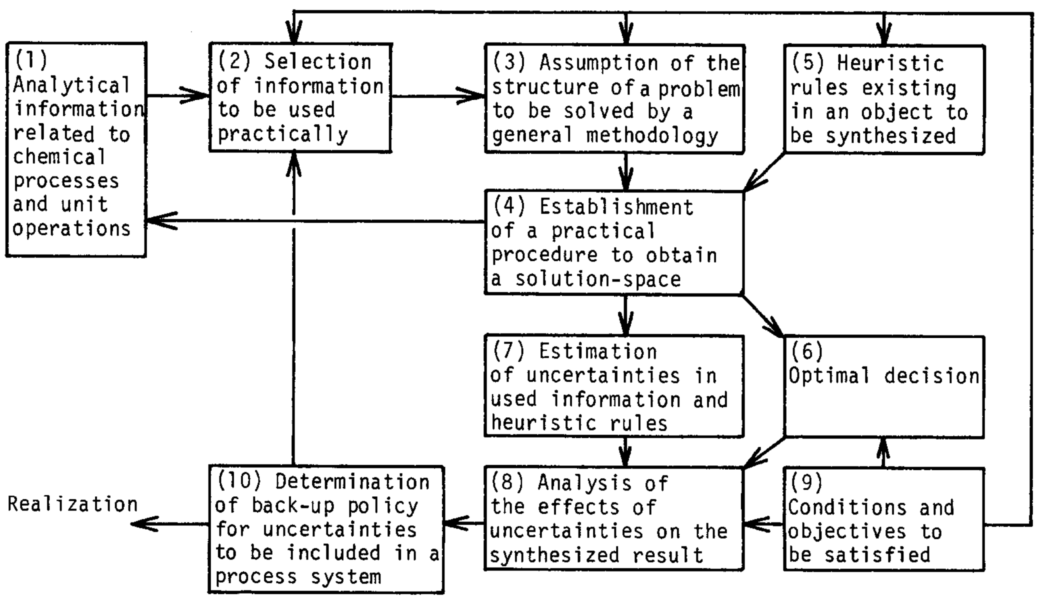


Fig. 5. A methodology of Process Systems Engineering for chemical processes

saving energy (Takamatsu and co-worker, 1981h), safety, operability, flexibility for the change of design conditions etc., be developed first. After that, the feature of the optimum solution for each individual objective is accumulated and integrated in order to obtain the optimum solution of an multi-objective problem.

As is well known, the development of electronic computers has been remarkable, allowing a tremendous amount of information to be processed in a very short time. Therefore, a chemical process is not only synthesized from the information on unit operations, but may also be synthesized directly from the information on basic physical, thermodynamic data and fundamental phenomena simultaneously with the synthesis of unit operations included in a chemical process to be synthesized. This tendency corresponds to a unification of Fig. 4 and Fig. 5 and has been promoted by the rapid development of computers. This way of thinking about synthesizing a chemical process might be practical and powerful. However, the idea that the problem for the synthesis of a chemical process is simply solved by using the integrated and processed information suitable to the synthesis, which may be obtained by analyzing the optimum solutions for unit operations, should not be neglected, especially from the academic point of view of Process Systems Engineering.

The status of Process Systems Engineering for chemical processes is not similar to that of unit operations, and the methodologies for each stage shown in Fig. 5 have not yet been established. Only the methodologies for synthesizing a process composed of the same kind of unit operations have, for the most part, been established and are applicable to the solution of practical problems. Summerizing the roles which Process Systems Engineering has played and has to play, the following conclusions may be reached:

(i) Effective methods for synthesizing a chemical process composed of the same kind of unit operations have been developed, for example to synthesize heat exchangers or distillation columns;

(ii) Many simulation programs have been developed and used practically in industry, but the characteristics and limitations of the usage of each program should be clear, and all programs should be classified based on performance;

(iii) A systematic method has to be developed about how to combine a general method and heuristic rules in an individual process;

(iv) In order to do the above, the analytical information for optimum solutions in the synthesis of unit operations must be accumulated and adjusted to be conveniently used to synthesize a chemical process; and finally

(v) Practical methods responsible for multi-objective problems have to be further developed, but at same time the accumulation and adjustment of the optimal solution for each individual objective are important.

## NEW TREND IN PROCESS SYSTEMS ENGINEERING

Process systems engineers still have so many problems to solve in the field of the design of unit operations and processes that it would almost seem impossible to solve them all to the point of practical usage in the near future. In spite of such a situation, however, these new problems must be faced and rapidly solved. Some of those problems are given in this section.

### Operational Problems in Chemical Processes

The core of Process Control has been established in the field of Chemical Engineering, and has contributed to the solution of certain operational problems for unit operations based on the application of classic control theories to unit operations. Recently, much research on the application of modern control theories to unit operations has been done. For example, there is research on multivariable control system design for a distillation column (Takamatsu and co-workers, 1974, 1978d, 1978f, 1979a, 1979c, 1981b, 1981e, 1981f), and on the application of a method for state estimation to the control of a fermentation process (Takamatsu and co-workers, 1979b, 1980a, 1981d). It seems, however, that there is no effective and general method except the "relative gain array method" to identify whether or not a modern process control system should be installed, prior to the system design. Modern process control systems, including electronic computers, will be widely and effectively used in many chemical processes, especially in multivariable and adaptive control systems, because a process control system design should be considered from the total process point of view rather than that of the control of a unit operation. The reasons why a control system design should be considered from the total process point of view are based on the facts that a chemical process becomes more and more complex by heat-integration for energy saving after which the interactions between unit operations become stronger. Also, a chemical process will be required to be adaptively responsible to changes in the quality and amount of the products. It is a very important problem to clarify the conditions under which modern control theories should be applied, such as what characteristics of an object to be controlled and how accurately the states of the object should be controlled.

Fig. 6 shows a general structure for solving operational problems. The meaning of each block may be easily understood if this figure is regarded as that for a conventional control system design. However, in so far as we recognize that the installation of a process control system for a unit operation is done to obtain better operational features for a chemical process, a synthesis for operational policy should be done, including the determination of a process control strategy, before the design of the process control system for a unit operation. As mentioned previously, I believe a separable hypothesis between design problems and operational problems cannot be ideally formed, especially if the synthesis of a back-up system for uncertainties in a process is considered. Therefore, in order to unify process design and operational problems, the methodology for the solution of the operational problems of the total process should be established. Moreover, operational problems have to include not only a steady state operation, but also start-up and shut-down operations as well as operations under abnormal conditions, such as accidents.

## Batch Process Systems Engineering

The importance of the unified consideration of design and operational problems has just mentioned, but the batch process has the strongest relationship to this point. So far Process Systems Engineering has developed for continuous chemical processes, but engineering on batch processes should also be established. Hereafter, the production of fine and special chemicals becomes probably more and more important, and these production processes, in general, have the characteristics of small amount and multi-product production with a large number of unit process steps. The production of these products often faces great changes in demand. Batch processes can easily correspond to conditions such as those just mentioned above. The rapid development and spread of micro-computers and robots must develop strong countermeasures to overcome the disadvantages of batch processes compared with continuous processes.

Recently, some research on Batch Process Systems Engineering have been reported, but much of it is concerned with developing computer programs to solve design and operational problems for batch processes. The establishment of Computer Aided Design and Scheduling is very important for practical applications, but the accumulation of basic logics and optimizing methods for the typical batch processes is also important (Takamatsu and co-workers, 1978g, 1981a). In the future, it will be desirable to develop Batch Process Systems Engineering including the control system design of a batch unit operation and the operation of storage tanks.

## The Challenge to Larger Process Systems

Some often say that theoretical or computational research may be meaningful only when the result or the assertion of the research can be confirmed by experiments or observations. This might be reasonable if an experimental consideration is practically possible for an object considered theoretically or numerically by computer simulation. It should be noticed, however, that a reasonable synthesis for a large process system which can not be experimentally confirmed is required in society, and the property of the large process system to the surroundings is often more critical than that of a small part in a system the characteristics of which can be confirmed

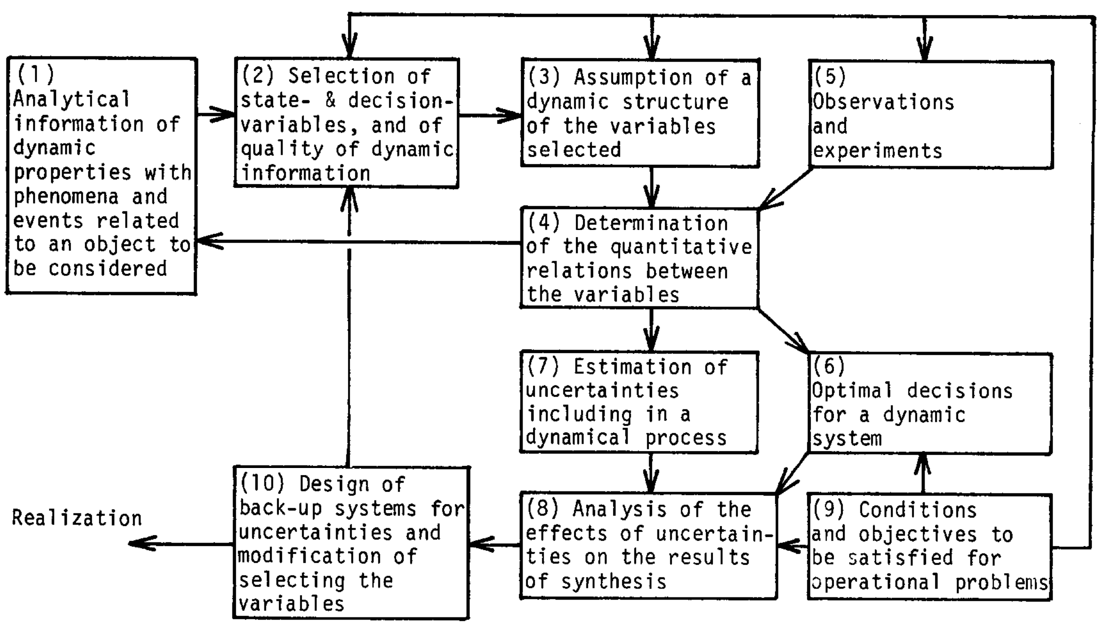


Fig. 6. A general structure to solve operational problems

by experiments. Although it is experimental, there is still the problem of how precise and useful experimental information is for practice.

It is recognized that Chemical Engineering contributes to the synthesis and analysis of phenomena, such as unit operation, process and system related to change, transfer and accumulation of mass and energy. Thus, process systems engineers have to be able to contribute to many industrial and national level's problems, such as planning for industrial structure, energy and resources policy at the national level (Takamatsu and co-workers, 1980b, 1981i; Yoshida and Takamatsu, 1981a, 1981b; Ohno and Takamatsu, 1981a, 198ab; Shioya and Takamatsu, 1981), and regional and national environmental assessment (Takamatsu and co-workers, 1969e, 1970d, 1970e, 1971c).

### The Challenge to the Creation of New Hard Systems

At the present time, there are no concrete methods to support the above title, but this title should not be forgotton by process systems engineers.

So far, Process Systems Engineering has been called a kind of "soft-engineering". That is, for example, consider the synthesis of a chemical process. It may be possible to obtain a new optimal configuration for unit operations. It might be said that this new configuration is a kind of new hard system, but it should really be called a new combination of given hard systems.

Since early times, it has been said that the usage of practical engineering systems has gone ahead in society, with academic solutions for the system having come later. This fact might be true at times when the major intention of natural science and engineering has been directed toward "Analysis". This is because "Analysis" cannot be done if the object does not exist in society. However, since the field of Process Systems Engineering is directed toward "Synthesis", the tradition that practical systems go ahead in the society is insufficient.

As far as it is possible to express matters and mechanisms in society as a combinations of an appropriate amount of information, it should be possible to express an ideal feature or the desirable condition of a system to exist only from the information. If this is so, the problem is how to change, transfer and accumulate the given information in order to achieve the relationships of information for an ideal feature. A new hard system might develop out of this conception.

## CONCLUSIONS

(1) "Learning is a search for truth" is a well known saying, but this tradition is liable to be understood only as applying to "Analysis". However, Process Systems Engineering has to progress in the direction of a search for the truth by "Synthesis".
(2) It is very valuable for engineering practice to be able to obtain an optimal solution by using a powerful electronic computer, but it is much better if the same solution can be simply obtained without using any computer.
(3) Therefore, although many methodologies for Process Systems Engineering have been developed, efforts must be made to analyze and adjust the optimal solutions obtained.
(4) So far, Process Systems Engineering has been mainly directed toward solving design problems, but operational problems have to be systematically solved by the establishment of a methodology as well. Also both design and operational problems should be unified in the future.
(5) A general extension of the above conclusion is the establishment of a methodology to solve multi-objective problems.
(6) It is necessary to meet the challenge of synthesizing larger and larger process systems and to create new hard systems.

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