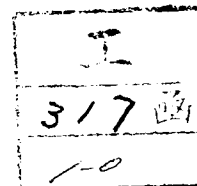


PROCESS SYSTEM IDENTIFICATION
AND OPTIMIZATION WITH PARAMETER UNCERTAINTY

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PROCESS SYSTEM IDENTIFICATION
AND OPTIMIZATION WITH PARAMETER UNCERTAINTY

by

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INTRODUCTION

Many engineering problems have been studied so that human life could be made richer and to improve present methods of production as well as to create new ones. These studies must be seen within their proper historical context in order that they be made more meaningful.

Sciences developed through a period when there was no distinct difference between scientist and engineer. As time passed, however, a large gap between engineering and natural science developed. In the early 20th century natural science developed as much as natural science could become the basis of engineering so that now, engineering is often spoken of as merely an application of natural science. This, however, is a mistake because of the following reason: It is impossible for natural science to completely encompass engineering despite the fact that natural science is a basis of engineering technology. If we want to apply a theory of natural science to some engineering technology, we cannot do so by trial and error, we need a high standard of creative ability.

The studies on process system identification and optimization, in which the studies by the author "Process System Identification

and Optimization with Parameter Uncertainty" is included, may be seen as a part of the field of engineering science^[0-1] that seeks to be a composite of natural science and engineering technology, a new field of engineering.

Two important tools of engineering science are mathematical analysis and numerical calculation. The most important starting point in the work of engineering is the recognition of the problem under study. We can start to analyse and compute mathematically until we recognize the problem. To recognize the problem is to answer the questions: "What is the problem?"; "What element is the most important one in the phenomena of the problem under study?" "What, if any, are the negligible elements of the problem?". To solve the problem of system optimization based on some recognition of the problem, three main steps are considered. See Fig.0.1.

First we must construct a model after we clearly recognize the problem. A model is a picture which is constructed by using every principal element and abbreviating every non-principal element identified through the understanding of the phenomena of the problem. We construct the model by simplification of phenomena based on our recognition of the problem by attaching importance to one phase of essential qualities of that phenomena.

There are two steps in system identification; (i) determination of the system model structure, and (ii) parameter estimation of the system. A brief introduction to system identification will be described in Chapter 1.

Secondly, we must calculate the optimal solution for the purpose of system synthesis based on the identified mathematical

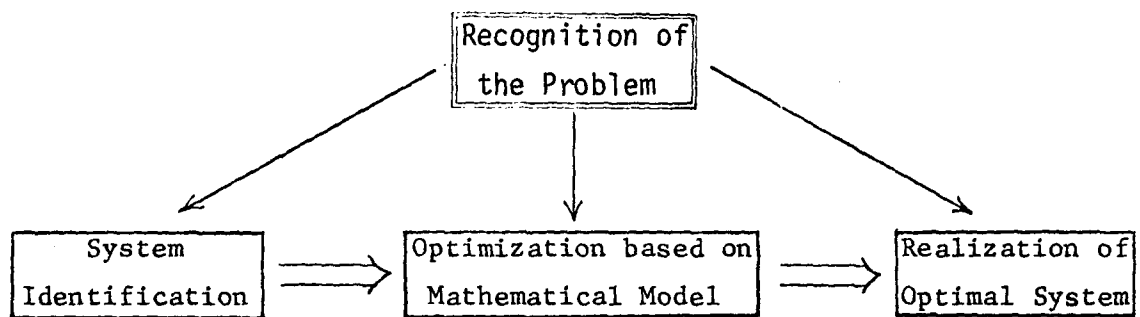


Fig. 0.1 Steps of Process System Optimization

model. In this step, various optimization techniques^{[0-3]~[0-50]}, for example, the Maximum Principle, Dynamic Programming, variational method, nonlinear programming, or various gradient methods, etc. can be used. A great many problems can be solved by using digital or analog computers.

Ultimately, we must realize the optimal solution of the system or synthesize optimal systems based on the calculated result. It will not always be sufficient to determine numerical optimal values based only on a mathematical model because such models are constructed by simplification of phenomena and thus contain various inevitable uncertainties. Finding the optimal solution or optimal system based on numerical solutions is the problem to be solved in this step.

In this paper, some problems of system identification and the realization of optimal systems with parameter uncertainty are studied having the purpose of synthesis in mind.

The results of these studies are applied to the design of a waste water treatment system.

Fig.0.2 is a list of the contents of each chapter of this paper. PART I is concerned with theoretical considerations, and PART II concentrates on an application to waste water treatment system design.

In Chapter 1, studies on model building and the application of sensitivity analysis to system synthesis with parameter uncertainty are briefly surveyed. In the literature^[0-61] by the author, an attempt is made to determine the model structure of a system. In Chapter 2, parameter estimation by the least square technique is

discussed when the model structure is given, and the geometrical meaning of the parameter estimation is indicated. In Chapter 3, a method of determining the experimental condition based on estimation error of parameters is presented. In Chapter 4, a method of evaluating the rational design margin taking into account parameter uncertainty is proposed and discussed. Moreover, various methods of design rationally taking into account parameter uncertainty are classified and discussed. In Chapter 5, an attempt to design a process system with parameter uncertainty by considering the movable ranges of manipulating variables is studied. Chapter 6 serves as an introduction to waste water treatment system design. In Chapter 7 and 8, models of the wet-air oxidation process of sludge which may be a subsystem of the waste water treatment system are determined and discussed experimentally using the result of Chapter 2. In Chapter 9, the rational design of a waste water treatment system is tried based on a mathematical model and the results of Chapter 4 and Chapter 5. In Chapter 10, the problem of time-dependent disturbance of input in an activated sludge system is discussed from the viewpoint of the static design of the system. At the end of the paper, the conclusions are presented. The contents of each chapter have been presented as follows by the author: Chapter 2^[0-51] Chapter 3^[0-52] Chapter 4^{[0-53],[0-54],[0-55]}, Chapter 5^[0-56], Chapter 7^[0-57], Chapter 8^[0-58], Chapter 9^[0-59], Chapter 10^[0-60].

* * * * *

Note; Nomenclature used and literature referred to in each chapter are listed in the end of that chapter.

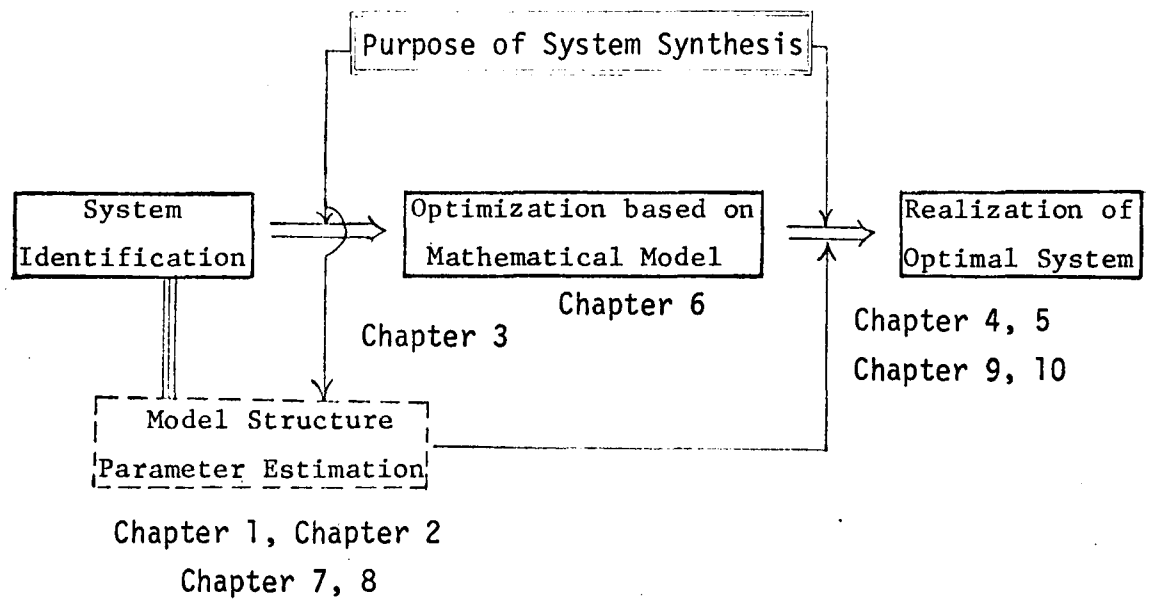


Fig. 0.2 Scope of the Thesis

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PART I

**SOME METHODOLOGIES FOR PROCESS SYSTEM IDENTIFICATION
AND OPTIMIZATION WITH PARAMETER UNCERTAINTY**

CHAPTER 1

SYSTEM IDENTIFICATION AND SENSITIVITY

1-1. SYSTEM IDENTIFICATION

1-1-1 Introductory Remarks

It may be useful for system synthesis to study system identification, or model building, in three steps as illustrated in Fig.

0.1. First, there is the problem of system identification. In recent years, aspects of system identification have been discussed in a multitude of survey papers [1-1]~[1-5] which we use here in our brief discussion of system identification.

It is often possible to perform experiments on a system in order to obtain the lacking knowledge. The final purpose of identification is to design a process system or plan a control strategy. One of the functions which undoubtedly contributed to the great success of frequency techniques in "classical" control theory was the fact that the design methods were accompanied by a very powerful techniques for systems identification, such as frequency analysis. This technique made it possible to determine transfer accurately, which is precisely what is needed to apply synthesis methods based

on logarithmic diagrams. The models used in "modern" control theory are, with few exceptions, parametric models in terms of state equations. The desire to determine such models from experimental data has naturally renewed the interest of control engineers in parameter estimation and related techniques.

The definition of an identification problem given by Zadeh [1-6] can be used as a starting point. An identification problem is characterized by three quantities; a class of models, a class of input singals, and a criterion. We have tried to emphasize this point of view.

When formulating and solving an identification problem it is important to have the purpose of the identification in mind. Models must be purpose-oriented. In process system engineering, the final goal is often to design a process system or to plan control strategies for a particular system. There are, however, also situations where the primary interest is to analyse the properties of a system. Determination of rate coefficients in chemical reactions, heat transfer coefficients of industrial processes and reactivity coefficients in nuclear reactors are typical examples of such a "diagnostic" situation. In such a case, determination of specific parameter values might be a goal of the identification, but the author wishes to emphasize that the final goal is system synthesis.

Formulation of identification problems

The following formulation of the identification problem given by Zadeh^[1-6] is still relevant; "Identification is the determination,

on the basis of input and output, of a system within a specified class of systems, to which the system under study is equivalent."

Using Zadeh's formulation, it is necessary to specify a class of systems, $S = \{S\}$, a class of input signals, U , and the meaning of "equivalent". In the following, we will call "the system under test" simply the process, and the elements of S will be called models. Equivalence is often defined in terms of a criterion or a loss function which is a function of the process output y_r and the model output y_m , i.e.

$$F = F(y_r, y_m) \quad (1.1)$$

Two models m_1 and m_2 are then said to be equivalent if the value of the loss function is the same for both models, i.e.

$$F(y_r, y_{m_1}) = F(y_r, y_{m_2}) \quad (1.2)$$

The selection of the class of models, S , the class of input signals, U , and the criterion are largely influenced by the a priori knowledge of the process as well as by the purpose of the identification. Then equivalence is defined by means of a loss function, the identification problem is simply an optimization problem; find a model such that the loss function is as small as possible.

The class of models S is called identifiable if the optimization problem has a unique solution. If S is defined as a parametric class, $S = \{S_\beta\}$, where β is a parameter, the identification problem then reduces to a parameter estimation problem. Such a formulation makes it possible to exploit the tools of estimation and decision theory. In particular, it is possible to use special estimation

methods e.g. the maximum likelihood method, Bayes' method or the mini-max method.

1-1-2 Classification of Identification Method

The different identification schemes that are available can be classified according to the basic elements of the problem, i.e. the class of systems S , the input signals U , and the criterion. Classification has been done extensively in Eykhoff^[1-3], Balakrishnan and Poterka^[1-4].

The class of Models S

Models can be characterized in many different ways: by non-parametric representations such as impulse response, transfer function, covariance functions, spectral densities, Volterra series and, by parametric models such as state models

$$\begin{aligned}\frac{dx}{dt} &= f(x, u, \theta) \\ y &= g(x, u, \theta)\end{aligned}\tag{1.3}$$

where x is the state vector, u the input, y the output, and θ a parameter (vector). It is known that the parametric models can give results with large errors if the order of the model does not agree with the order of the process. The nonparametric representation has the advantage of not being necessary to specify the order of the process explicitly. These representations are, however, intrinsically infinite dimensional which means that it is frequently

possible to obtain a model such that output agrees exactly with the process output.

Needless to say, the models must be judged with respect to the ultimate aim.

The class of input signals

It is well known that significant simplifications in the computations can be achieved by choosing input signals of a special type e.g. impulse function, step functions, and white noise, etc.. Bibliographies on the use of these signals are given in Nikiforuk and Gupta^[1-7], Strobel^[1-8], Gitt^[1-9], Wilfert^[1-10].

The criterion

The criterion is often a minimization of a scalar loss function. The loss function is chosen, and the identification problem is formulated as an optimization problem.

Mostly the criterion is expressed as a functional of an error, e.g..

$$F(y_r, y_m) = \int_0^T e^2(t) dt \quad (1.4)$$

where y_r is the process output, y_m , the model output, and e , the error; y_r, y_m and e are considered as functions defined on $[0, T]$. Notice that criterion (1.4) can be interpreted as a least squares criterion for the error e . The case

$$e = y_r - y_m \quad (1.5)$$

is referred to as the output error. On the otherhand, the input error[1-5], [1-11] or generalized error[1-12] may be taken as the error $e..$

Computation Aspects

All solutions to parametric identification problems consist of finding the extremum of the loss function F considered as a function of the parameters θ . The minimization can be done in many different ways e.g.,

(i.) as a "one-shot" approach, i.e. solving the relations that have to be satisfied for the extremum of the function or functional; or
(ii.) as an interactive approach, i.e. by some type of steepest ascent method. In this case, numerous techniques are available, e.g.

a.) cyclic adjustment of the parameters one-by-one, e.g. the Southwell relaxation method

b.) gradient method:

$$\theta(i+1) = \theta(i) - \lambda F_{\theta}(\theta(i)) \quad \lambda > 0 \quad (1.6)$$

$$\lambda = \text{constant}$$

F_{θ} is a partial derivative of F with respect to θ^* .

c.) steepest descent method:

$$\theta(i+1) = \theta(i) - \lambda(i) \cdot F_{\theta}(\theta(i)) \quad (1.7)$$

$\lambda(i)$ chosen such that $F(\theta)$ is minimum in the direction of the gradient.

d.) Newton's method

$$\theta(i+1) = \theta(i) - \lambda(i) \cdot F_{\theta}(\theta(i)) \quad (1.8)$$

$$\lambda(i) = [F_{\theta\theta}(\theta(i))]^{-1}$$

e.) conjugate gradient method

$$\theta(i+1) = \theta(i) - \lambda(i) \cdot d(i) \quad (1.9)$$

$$d(i) = F_{\theta}(\theta(i)) - \frac{F_{\theta}(\theta(i))^2}{F_{\theta}(\theta(i-1))^2} \quad (1.10)$$

$\lambda(i) > 0$ minimizes $F(\theta(i) - \lambda d(i))$

This method is called as the Fletcher-Reeves's method.

The Davidon Fletcher-Powell's method is introduced in Chapter

2. This method, applied to a positive definite quadratic function of n variables, can reach the minimum in at most n steps.

In these method the practice of estimating the determination of the gradient which is degraded through the stochastic aspects of the problem has not been taken into account. A method which considers this uncertainty in the gradient-determination is the:

f.) stochastic approximation method:

$$\theta(i+1) = \theta(i) - \lambda(i) F_{\theta}(\theta(i)) \quad (1.11)$$

where $\lambda(i)$ has to fulfill the conditions^[1-5]

$$\lambda(i) \geq 0$$

$$\sum_{i=1}^{\infty} \lambda^2(i) < \infty \quad \sum_{i=1}^n \lambda(i) \rightarrow \infty \text{ as } n \rightarrow \infty$$

As an example $\lambda(i) = 1/i$ may be used.

Good surveys of optimization techniques have been found in the books by Wilde^[1-13], and a by Bekey and McGee^[1-14].

1-1-3 Choice of Model Structure

The choice of model structure is one of the basic ingredients in the formulation of the identification problem. The choice will greatly influence the character of the identification problem. There are very general results available with regard to the choice of structure^[1-5]. These results are mainly referred to as the minimal realization of the linear system^{[1-15]~[1-25]}. We won't discuss this general problem here. In the literature, however, we discuss the selection of the model structure of a process system for a special case when the system is nonlinear^[0-61].

1-1-4 Parameter Estimation in Parametric Models

After we select the model structure in parametric model system, we must estimate the parameters included in the model. Parameter estimation in ordinary differential equations and linear algebraic equations will be discussed in Chapter 2.

We have mentioned briefly the applicable identification problem and its techniques, however, there are many important questions that remain to be answered. See [I-26]~[I-86].

1-2. SYSTEM SENSITIVITY

1-2-1 Sensitivity in System Synthesis

The concept of sensitivity was discussed about ten years ago [1-87]~[1-96], and several papers about the development of this field have appeared [1-97]~[1-107]. We now briefly describe recent developments in the field, especially with respect to application of sensitivity to system synthesis and identification.

The study of sensitivity in the field of system optimization has been studied according to various concepts. K. Inoue and I. Hashimoto classify these studies in dynamic systems into four categories: (i) sensitivity constrained optimal control, (ii) optimally sensitive control, (iii) application to parametric optimization, and (iv) others [1-108]....

Another point of view in classifying the studies of sensitivity as applied to system synthesis is on design margin or rational design of the static system with uncertain parameters. The classification and comparison of studies from this point of view are shown in Chapter 4. We summarize the recent studies of sensitivity on dynamic systems by classifying the four categories described above as follows:

(i) Sensitivity Constrained Optimal Control

Sensitivity constrained optimal control is to synthesize optimal control so as to make the system insensitive for parameter deviation and uncertainty. For this purpose, a new model system composed of the original system equations and sensitivity equations [1-109]~[1-112] are considered.

Based on new objective functions including a sensitivity

function (modified performance index) or new constraint, optimal control is determined. The three main criteria are as follows; (a) reduction of trajectory sensitivity^{[1-113]~[1-115]} (b) reduction of the sensitivity of the terminal value of the state variable^{[1-116] [1-118]}, and (c) reduction of the sensitivity of the performance index^[1-119].

(ii) Optimally Sensitive Control

Optimally sensitive control^[1-120] is to determine quasi-optimal control as follows:

Optimal control is considered as a function of the parameter.

Based on the approximation by Taylor Series expansion, quasi-optimal control^{[1-121]~[1-123]} in the neighborhood of the nominal value may be determined by simple calculation. By first order approximation of Taylor Series expansion of the optimal control $u(t)$, the following equation

$$\tilde{u} = u^* + w\rho^{-1}(\tilde{x} - x^*) + (\gamma - w\rho^{-1}\sigma)\Delta q \quad (1.12)$$

$$\tilde{u} = u^* + \gamma\sigma^{-1}(\tilde{x} - x^*) + (w - \gamma\sigma^{-1}\rho)\Delta x^0 \quad (1.13)$$

where w, ρ, γ are sensitivity functions which are given as the solution of ordinary differential equations^[1-120]. The concept of the optimally sensitive control is applied to

description in given in reference^[1-108].

(iv) Others

The method of determining control u by minimizing respective sensitivity of the performance index^{[1-140]~[1-144]} has been proposed. The idea cannot be classified into these three categories however.

1-2-2 Sensitivity in Process System Design

[a] Accounting for uncertainty in data

In process system design, there are many uncertainties, e.g. a variation in environmental conditions, the rate of a reaction in a proposed reactor, or the efficiency of a separation process. We must establish a strategy for hedging against design errors caused by this persistent uncertainty.

The process engineer protects his system from the effects of uncertainty in design data by engineering on the "safe side". In many situations, the processing components are purposely designed to be more durable, more flexible, and of greater capacity than is needed on the basis of the best information available, in an attempt to protect the system from unknown effects. On the otherhand, when the uncertainty surrounds a critical feature of a novel system, the engineer may elect not to gamble on a full scale design and may recommend the construction of a small scale pilot plant to test the processing concept, thereby putting less capital investment in jeopardy. An overdesign of from 11 to 24 per cent commonly has been used mostly to hedge against errors in the basic data and equations. The evidence upon which such general overdesign factors are based

is generally quite tenuous, and such factors must be considered more as articles of faith than reason. In nearly all processing problems, certain bits of information are critical in the sense that small changes in the values assumed by those critical parameters greatly influence the solution to the problem.

The sensitivity of the design equations to changes in parameters can be tested by incrementing each parameter in turn and computing the effect on the system of this change.

There is a natural human tendency to ignore factors which are not well understood and to attempt to avoid basing decisions on partial or conflicting information. Unfortunately, in process engineering, uncertainties crop up in the most critical portions of problems, and frequently there is not enough time to undertake an elaborate scientific study to reduce them.

The empirical art of overdesign was evolved to provide some measure of security in this naturally insecure area.

[b] Application of sensitivity analysis to design

Design margin taking into account such parameter uncertainties as described above, primarily from the viewpoint of sensitivity analysis, has been studied. The application of sensitivity analysis to process system design also has been studied^{[1-145]~[1-168]}, and are described in Chapter 4 and 5.

1-2-3 Sensitivity in System Identification

As stated in 1-1-2, sensitivity method is applied to system parameter identification, and is described briefly once more here. System parameter identification methods are classified as follow:

One shot method

{ Inverse Sensitivity Method^{[1-97],[1-169]}
Pseudo-Sensitivity Method^[1-170]
Determination of nominal parameter value

Iterative method

{ Gradient Method^[1-171]
Newton-Raphson Method, Gauss-Newton Method^{[1-172],[1-173]}
Observer Method

Another application of the sensitivity method to system parameter identification is when the optimal input (or experimental conditions) is determined so as to pin point the parameter value more precisely [168],[174]~[1-176]. The studies of system identification from the viewpoint of sensitivity method may be necessary in the future.

NOMENCLATURE

e ; error between model and system

S ; class of system

U ; class of input signal

u ; input variables

x ; state variables

y_m ; model output

y_r ; system output

θ ; parameters included in parameteric model

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CHAPTER 2

PARAMETER ESTIMATION BY LEAST SQUARE TECHNIQUES

2-1. INTRODUCTORY REMARKS

In most engineering situations, the black box approach is not a very realistic one. The experimenter, in many cases, has derived some prior knowledge from physical insight into the process under consideration. This may give information on the topology of a conceptual model for that process, and perhaps even an approximate knowledge on the values of the parameters in that model. On account of the wide variety of different "processes" for which models have to be built (the range includes high performance aircraft as well as chemical production plants), model building is quite strongly object-oriented.

In this chapter, we will consider the problem of parameter estimation by least square estimation. That is, the model structure is given beforehand and the estimation of the parameter value is the problem considered here. For simplicity, the model structure may be assumed to be linear with respect to the parameter if neces-

sary. The parameter estimation problem can be represented by the block diagram Fig.2.1 where P is the process with parameters b, and M is a conceptual model with parameters β ; [2-1]

Consequently,

$$z = y(b) + n \quad (2.1)$$

$$w = U\beta \quad (2.2)$$

with

$$U = (u_1, \dots, u_m) = \begin{vmatrix} u_1(0), \dots, u_m(0) \\ \vdots \\ u_1(k\tau), \dots, u_m(k\tau) \end{vmatrix}$$

where, $b' = \{b_1, \dots, b_n\}$

$\beta' = \{\beta_1, \dots, \beta_n\}$

$z' = \{z(0), z(\tau), \dots, z(k\tau)\}$

and ' denotes the transposition of a vector.

Now one can define the problem as the task of finding the best estimate β of the process parameters b, based on observation of z. In the statistical literature, a number of different estimation procedures have been developed. These methods differ predominantly in the criteria used for defining optimality and in the use of available prior knowledge. It is unfortunate that the choice between these criteria has aspects that are more or less subjective and that the mathematical approach is strongly dependent on these criteria.

Our interest lies primarily in :

1) The minimization of some function of $\beta-b$, the difference between

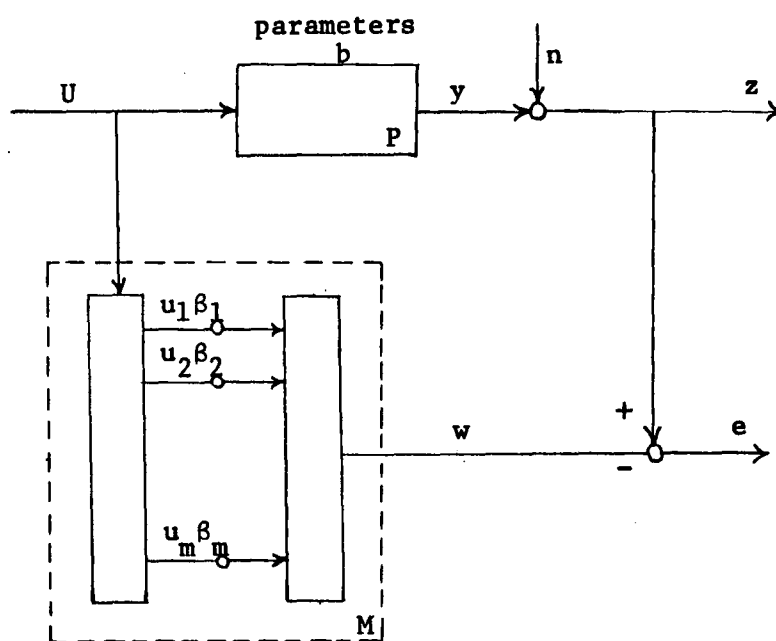


Fig. 2.1 Comparison of the process with an adjustable model.

the process parameter vector b and its estimate β . As b is inaccessible for direct measurements, we can only minimize the expectation of this difference if sufficient priori knowledge is available.

2) The minimization of some functional or function of $e = z - w = z - U\beta$, the error between the output of the process and the output of a conceptual model. If this model can represent the process behaviour completely, i.e. if

$$y = U\beta \quad (2.3)$$

then

$$e = U(b - \beta) + n \quad (2.4)$$

Consequently "e" can provide some measure of the correspondence of the parameter vectors. This error may be used because "e" can be made measurable and because in some cases, the correspondence of input-output relations is more important than parameter correspondence, particularly if the model is simpler (e.g. of lower order) than the process.

3) The minimization of some functional containing the measurable process outputs and the unknown estimates of process state vector and the process parameter vector.

In this chapter, we describe briefly statistical estimation theory and make clear the meaning of least square parameter estimation. Next, the mathematical background and the geometric meaning of parameter estimation by the least square method are given. Finally, an estimation technique by the DFP method is described as a method of solving the parameter estimation problem.

2-2. STATISTICAL ESTIMATION THEORY

The parameter estimation cases to be considered are illustrated in Fig.2.1. We want to derive an estimate, i.e. a fundamental relationship

$$\beta_i = \beta_i\{z(0), \dots, z(k\tau)\} = \beta_i(z) \quad (2.5)$$

so that a numerical value can be assigned for the process parameter β_i from the sequence of observations on the output signal z .

When a number of parameters $\{\beta_1, \dots, \beta_m\} = \beta'$ have to be estimated, the relationship is indicated by $\beta = \beta(z)$.

In the statistical literature, e.g. ref.[2-2], some properties are defined for such functional relationships as :

- i) unbiased estimate : if $E[\beta] = b$
- ii) efficient estimate : $\beta(z)$ is an efficient estimate if
$$E[(\beta-b)^2] \leq E[(\gamma-b)^2] \text{ for all } \gamma = \gamma(z)$$
- iii) consistent estimate : $\lim_{k \rightarrow \infty} p\{(\beta-b)=0\} = 1$

where $E[\]$ denotes the mathematical expectation. The first two properties may also hold only for $k \rightarrow \infty$, in that case they are called asymptotic unbiasedness and efficiency.

As a starting point for deriving estimates we will choose a situation where much prior knowledge is available^[2-3], viz. :

- (a) The probability density function of the noise n . From this function the probability density of the measurements z follows; This function, being dependent on the process parameters b , is denoted as $p(z|b)$.
- (b) The probability density functions of the parameter values b ;

This function is written as $q(b)$.

- (c) The cost of choosing the value β for the estimate if the true value of the process parameter is b . This cost or loss function $C(\beta, b)$ has a minimum for $\beta=b$.

After considering the use of all this information, we will indicate the effect of dropping the assumptions (c), (b) and (a) successively.

[I] The conditional risk of choosing $\beta(z)$ if the true process parameter value is b can be written as the expectation of the cost function with respect to the probability of the observations z :

$$E_z[C(\beta, b)|b] = \int_{k+1} C(\beta, b) \cdot p(z|b) d^{k+1}z \quad (2.6)$$

where the following notation is used :

$E_z[\]$ is the expectation with respect to z

$\int_{k+1}$ indicates an $k+1$ fold integral

$$d^{k+1}z = dz(0)dz(\tau) \dots dz(k\tau)$$

The average risk for this estimating situation is the expectation with respect to the probability of the values of the parameter b

$$R(\beta) = E_b[E_z[C(\beta, b)|b]] = \int_m \int_{k+1} C(\beta, b) p(z|b) q(b) d^{k+1}z \cdot d^m b, \quad (2.7)$$

The estimate that minimizes this expression is called the minimum risk, minimum cost, or Bayes estimate. Due to the well known relationships as follow ;

$$p(z|b)q(b) = p(z, b) = p(b|z)p(z) \quad (2.8)$$

the average risk can be written as :

$$R(\beta) = \int_{k+1} d^{k+1} z \cdot p(z) \int_m C(\beta, b) p(b|z) d^m b \quad (2.9)$$

Since $p(z) > 0$, the average risk $R(\beta)$ can be minimized by making the second integral as small as possible for each z :

$$\text{Min}_{\beta} \int_m C(\beta, b) p(b|z) d^m b \quad (2.10)$$

A necessary condition for such a minimum is simply :

$$\frac{\partial}{\partial \beta} \left\{ \int_m C(\beta, b) p(b|z) d^m b \right\} = 0$$

As $C(\beta, b)$ has a minimum for $\beta=b$, as it presumably is small for values of β in the vicinity of b , and since

$$\int_m p(b|z) d^m b = 1 \quad (2.12)$$

it will be clear that equation (2.10) is satisfied if β is chosen in the neighbourhood of the b where the conditional probability $p(b|z)$ is maximum.

[II] Now we will drop assumption (c) i.e. the knowledge about an adequate cost or loss function $C(\beta, b)$. In that case, it is reasonable to choose β at that value of b for which $p(b|z)$ is a maximum. According to Eq.(2.8) :

$$p(b|z) = \frac{p(z|b)q(b)}{p(z)} \quad (2.13)$$

with

$$p(z) = \int_m p(z|b)q(b) d^m b$$

both assumption (a) and (b) are still being used.

[III] Next, we will consider the cosequences of dropping both assumptions (b) and (c) ; the a priori probability, $q(b)$ of the process parameters b is unknown. This ignorance can be expressed by assuming a uniform distribution $q(b)=\lambda$ over the interval under consideration. In that case, for any z ,

$$\text{Max}_b \{p(b|z)\} = \frac{\lambda}{p(z)} \text{Max}_b \{p(z|b)\} \quad (2.14)$$

As b is no longer a random variable but an unknown constant parameter, the following necessary conditions for finding the maximum can be given as,

$$\frac{\partial}{\partial b} p(z;b) = 0 \quad (2.15)$$

or as the logarithmic function is monotonic,

$$\frac{\partial}{\partial b} \ln p(z;b) = 0 \quad (2.16)$$

Picking that root of this set of equations which yield the largest value for $p(z;b)$ we have obtained the celebrated maximum likelihood estimate (M.L.E.) [2-1]

Now let us refer again to Fig.2.1 and assume that n has a $k+1$ variate Gaussian distribution i.e.

$$p(n) = \frac{1}{(2\pi)^{(k+1)/2} |N|^{1/2}} \exp\left[-\frac{1}{2} n' N^{-1} n\right] \quad (2.17)$$

with

$$E[n] = 0, \quad E[nn'] = N$$

Then we can write for the logarithm of the probability density

function of $n=z-U\beta$,

$$\ln p(z-U\beta) = -\frac{1}{2}\ln\{(2\pi)^{k+1}|N|\} - \frac{1}{2}\{(z-U\beta)'N^{-1}(z-U\beta)\}, \quad (2.18)$$

maximizing this function leads to ;

$$\frac{\partial}{\partial \beta}\{(z-U\beta)'N^{-1}(z-U\beta)\} = 0 \quad (2.19)$$

or

$$U'N^{-1}U\beta - U'N^{-1}z = 0 \quad (2.20)$$

If $U'N^{-1}U$ has an inverse, then Eq.(2.20) can be written,

$$\beta = (U'N^{-1}U)^{-1}U'N^{-1}z \quad (2.21)$$

This is the expression for the Markov estimate.

[IV] If knowledge on the covariance matrix of the noise is also lacking, it is best to choose $N^{-1}=I$, the identity matrix, assuming that the noise is white. Consequently,

$$\beta = (U'U)^{-1}U'z \quad (2.22)$$

This is the expression for the least squares estimate.

The Markov and least square estimate have been derived from the maximum likelihood estimate under the assumption of Gaussian noise. This has only been done to indicate the type of relationship that exists between the different estimates. These estimates, however, can be derived irrespective of the type of probability distribution of the noise by minimizing respectively the conceptual errors, cf. :

$$E = e'N^{-1}e \quad (2.23)$$

and

$$E = e'Ie = e'e \quad (2.24)$$

with

$$e = z - U\beta$$

Some of the relations between the different types of estimates are summarized in Table 2.1.

Table 2.2 Summary of the Different Estimates.

	Bayes estimation	Unconditional maximum likelihood estimation	Conditional maximum likelihood estimation	Markov estimation	Least squares estimation
2. Apriori Knowledge	$p(z b)$ $q(b)$ $C(\beta, b)$	$p(z b)$ $q(b)$	$p(z;b)$	$N = \epsilon[n \cdot n']$	Nil
Conditions	$\min_{\beta} \int C(\beta, b) p(b z) d^m b$	$\max_b p(b z) =$ $= \max_b \frac{p(z b)q(b)}{p(z)}$	$\max_b p(z;b)$ or $\max_b \ln p(z;b)$	$\tilde{\beta} = (U'N^{-1}U)^{-1}$ $U'N^{-1}Z$	$\tilde{\beta} = (U'U)^{-1}U'Z$
Properties	min. risk or cost		asympt. normality asympt. unbiased asympt. efficient (min, variance)	linearity unbiasedness	linearity unbiasedness
Relations			If gaussian noise		If white noise

2-3. MATHEMATICAL BACKGROUND FOR LEAST SQUARE PARAMETER ESTIMATION

2-3-1 General Remarks

The problem of the parameter fitting can be discussed generally because the problem is reduced to the optimal problem. There are many papers on this subject, for example, those by G.E.P. Box^[2-5] [2-15], and others^[2-16] [2-36]. In this section, the mathematical background and the geometric images of parameter fitting are given.

The problem of the parameter fitting becomes the optimal problem for the example as follows :

The process equations are

$$\dot{x} = f(x, \theta, t), \quad x(0) = x_0 \quad (2.25)$$

where, x is n -dim. column state vector, θ is p -dim. unknown parameter vector and " $\dot{\cdot}$ " denotes the first derivative with respect to the time t . The observed equations at time t_i are

$$y_i = g[x(t_i)] + \eta_i \quad i = 1, \dots, r \quad (2.26)$$

where, y_i are m -dim. column, observed value vectors, and η_i are m -dim. column error vectors. At this time, find the parameters minimizing the performance index $F(\theta)$ in Eq.(2.27) subjected to Eq.(2.25) and Eq.(2.26),

$$F(\theta) = \sum_{i=1}^r (y_i - g[x(t_i)])' \cdot W_i \cdot (y_i - g[x(t_i)]) \quad (2.27)$$

where W_i is $m \times m$ weighting matrix and "'" denotes transposing of the vector.

This performance index means that the observed error is

minimized. But there are questions as to how the weighting matrix W_i is chosen and what meaning the estimated value $\bar{\theta}$ minimizing $F(\theta)$ has. These questions are discussed below.

2-3-2 Statistical Treatment of Parameter Fitting

(1) Least square estimation

In this chapter it is assumed that the structure of the model is known already, and the discussion proceeds based on the following assumptions :

- Assumption I
- (i) The relations between the variable x , that is to say, the process equations are known.
 - (ii) The value of the state variables cannot be observed directly. Instead of this, the value of known function of x can be observed.
 - (iii) The observed value y contains the random error η .
 - (iv) The observed error η is contained as the added form. If it is not, it is assumed that y is expanded in Tayler series with respect to η and approximated by the first order of η .

Moreover the statical properties of the η are known. Next, let's define the problems of the linear and nonlinear parameter fittings.

The problem of the linear parameter fitting :

First, the observed equations are,

$$y = X \cdot \theta + \eta \quad (2.28)$$

y and η are as follow,

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix}, \quad \eta = \begin{bmatrix} \eta_1 \\ \vdots \\ \eta_r \end{bmatrix} \quad (2.29)$$

where, y_i : m-dim. column known observed value vector,

η_i : m-dim. column error vector,

θ : p-dim. column unknown parameter vector,

X : $n \times p$ known matrix constructed by state variables,

and $m \times r = n$, that is to say, y and η are n -dim. vector. Then, the

problem of linear parameter fitting is to find the parameter value $\bar{\theta}$ minimizing the following performance index $F(\theta)$

$$F(\theta) = (y - X \cdot \theta)' \cdot W \cdot (y - X \cdot \theta) \quad (2.30)$$

subjected to Eq.(2.28). Where, in Eq.(2.30), the $n \times n$ weighting matrix W is

$$W = \begin{bmatrix} W_1 & & & 0 \\ & \ddots & & \\ & & \ddots & \\ 0 & & & W_r \end{bmatrix} \quad (2.31)$$

and W_i is a $m \times m$ weighting matrix for all i .

The problem of the nonlinear parameter fitting :

The process equations are

$$\dot{x} = f(x, \theta, t) \quad x(0) = x_0, \quad (2.32)$$

where, x is l -dim. column state vector,

θ is p -dim. column unknown parameter vector,

f is the known function.

And the observed equations are

$$y_i = g[x(t_i)] + \eta_i \quad i=1, \dots, r \quad (2.33)$$

where, y_i is m-dim. known observed column vector,

η_i is m-dim. error column vector,

g is known function.

Here for simplicity, Eq.(2.33) is rewritten as follows,

$$y = g(x) + \eta \quad (2.33)'$$

where,

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix}, \quad \eta = \begin{bmatrix} \eta_1 \\ \vdots \\ \eta_r \end{bmatrix} \quad \text{and} \quad g(x) = \begin{bmatrix} g[x(t_1)] \\ \vdots \\ g[x(t_r)] \end{bmatrix}$$

Of course y and η are both n-dim. column vectors.

Then the problem of the nonlinear parameter fitting is to find the parameter value $\bar{\theta}$ which minimizes the performance index $F(\theta)$ as follows,

$$F(\theta) = (y - g(x))' \cdot W \cdot (y - g(x)) \quad (2.34)$$

subjected to Eq.(2.32) and Eq.(2.33)', where in Eq.(2.34) $n \times n$ weighting matrix W is the same as shown in Eq.(2.31). Then, $F(\theta)$ can also be rewritten as follows,

$$F(\theta) = \sum_{i=1}^r (y_i - g[x(t_i)])' \cdot W_i \cdot (y_i - g[x(t_i)]) \quad (2.34)'$$

Now, the policy of parameter fitting is to seek the parameter which minimizes the sum of the squares of observed error. This is

called the least square estimation. Then, the following assumption is adopted with respect to the random observed error η :

Assumption II (i) η_i has a Gaussian distribution with zero mean and with the covariance matrix M_i ,

(ii) η_i and η_j are statistically independent.

Based on Assumption II, the least square estimation is considered reasonable. Furthermore, using the same assumption if W_i is taken as M_i^{-1} , this policy becomes the maximum likelihood estimation, where M_i^{-1} denotes the inverse matrix of M_i . This fact is explained as follows : From Assumption II, the probability density $p(\eta_i)$ of η_i is represented as,

$$P(\eta_i) = \frac{1}{(2\pi)^{\frac{m}{2}} \sqrt{|M_i|}} \exp\left\{-\frac{1}{2} \eta_i' \cdot M_i^{-1} \cdot \eta_i\right\} \quad (2.35)$$

Because η_i and η_j are statistically independent ($i \neq j$), the maximum likelihood function $L(\eta_1, \dots, \eta_r)$ becomes,

$$L(\eta_1, \dots, \eta_r) = \prod_{i=1}^r P(\eta_i) = \frac{1}{\prod_{i=1}^r (2\pi)^{\frac{m}{2}} \sqrt{|M_i|}} \exp\left\{-\frac{1}{2} \sum_{i=1}^r \eta_i' \cdot M_i^{-1} \cdot \eta_i\right\} \quad (2.36)$$

Minimizing $L(\eta_1, \dots, \eta_r)$ is to minimize L shown as

$$L = \sum_{i=1}^r \eta_i' \cdot M_i^{-1} \cdot \eta_i \quad (2.37)$$

If W_i is chosen as M_i^{-1} , from Eq.(2.33), (2.34) and (2.37), the performance index of the least square estimation is equal to one of the maximum likelihood estimation. From this result, W_i is

chosen as M_i^{-1} for all i hereafter, and M^{-1} is defined as,

$$M^{-1} = \begin{bmatrix} M_1^{-1} & & 0 \\ & \ddots & \\ 0 & & M_r^{-1} \end{bmatrix} \quad (2.38)$$

W is taken as

$$W = M^{-1} \quad (2.39)$$

where M is symmetrical and positive definite. From the above discussion, it can be seen that the least square estimation is reasonable.

(2) Parameter confidence region

In both cases, linear parameter fitting and nonlinear parameter fitting, the observed value y contains the random error η . Therefore, the estimated parameter value $\bar{\theta}$ using the observed value y must be seen as a probabilistic variable. That is to say, the estimated parameter value $\bar{\theta}$ by using a class of observed values cannot always be coincident with the true parameter value θ^* . Only the information with respect to the true parameter value θ^* that the true parameter value θ^* will fall in some interval or regions in a specified proportion of the occasion which we determine is given. This region in a specified proportion of occasions is called "the parameter confidence region". For example, if Σ is the 95[%] confidence region, the statement that θ^* is in Σ will be true, on an average of 19 times out of 20. Furthermore, the size of the confidence regions will be the measure of the accuracy of the estimated parameter value $\bar{\theta}$. From these, the parameter

confidence regions as well as the estimated parameter value $\bar{\theta}$ is the important factor of the parameter fitting.

Let's now consider how the parameter confidence region is represented in linear and nonlinear parameter fitting, respectively. We assume that W is chosen as Eq.(2.39) in the linear parameter fitting. In a nonlinear parameter fitting, we assume that W is chosen arbitrarily as a general rule, and that initial condition x_0 must be estimated.

(a) In the case of a linear parameter fitting :

In the case of a linear parameter fitting, the estimated parameter value satisfies the following equation,

$$X^T M^{-1} \cdot X \cdot \bar{\theta} = X^T M^{-1} \cdot y \quad (2.40)$$

which is called the normal equation. Eq.(2.40) is derived from Eq.(2.28), Eq.(2.30) and $\partial F(\theta)/\partial \theta = 0$. Now, it is assumed that the estimated parameter value $\bar{\theta}$ is close to the true value θ^* , and θ^* is represented as $\theta^* = \bar{\theta} + \Delta\theta$. Then, from Eq.(2.28) and Eq.(2.40),

$$X^T M^{-1} \cdot X \cdot \Delta\theta = -X^T M^{-1} \cdot \eta \quad (2.41)$$

From this equation it is seen that $\Delta\theta$ has a Gaussian distribution with zero mean. Then the variance of Eq.(2.41) is given

$$E(X^T M^{-1} \cdot X \cdot \Delta\theta \cdot \Delta\theta^T \cdot X^T M^{-1} \cdot X) = E(X^T M^{-1} \cdot \eta \cdot \eta^T \cdot M^{-1} \cdot X) \quad (2.42)$$

Therefore, the variance of the $\Delta\theta$ is given as

$$E(\Delta\theta \cdot \Delta\theta^T) = V(\Delta\theta) = (X^T M^{-1} \cdot X)^{-1} \quad (2.43)$$

If M equals unit matrix I , from statistical theory, the confidence

region of the $\bar{\theta}$ on the level $(1-\alpha)$ is given by using Eq.(2.43) as follows^[2-21],

$$\Delta\theta \cdot \hat{X}'X \cdot \Delta\theta \leq p \cdot S^2 \cdot F(p, n-p, 1-\alpha) \quad (2.44)$$

where $I \cdot S^2$ is the mean square of η , and $F(p, n-p, 1-\alpha)$ is a F-distribution with degree of p and $n-p$ on level $(1-\alpha)$. The $(1-\alpha)$ confidence regions are given as,

$$(\theta^* - \bar{\theta})' \hat{X}'X (\theta^* - \bar{\theta}) \leq p \cdot S^2 \cdot F(p, n-p, 1-\alpha) \quad (2.45)$$

Hence if we assert that Eq.(2.45) is satisfied, then, in a large number of similar experiments, we shall be correct on $(1-\alpha)$ of the occasions.

(b) In the case of nonlinear parameter fitting :

Now we assume that weight W is an arbitrary value and that x_0 must be also estimated in the same way as parameters. It is assumed that the parameter value which minimizes the $F(\theta, x_0)$ in Eq.(2.34) is $(\bar{\theta}, \bar{x}_0)$. When the deviations of the parameter and initial condition are given as $\Delta\theta$ and Δx_0 , respectively, the following conditions must be satisfied,

$$\frac{\partial F}{\partial \theta} = -2(y - g(x))' W \cdot G \cdot \lambda = 0 \quad (2.46)$$

$$\frac{\partial F}{\partial x_0} = -2(y - g(x))' W \cdot G \cdot X = 0 \quad (2.47)$$

where,

$$G \triangleq \left| \frac{\partial g(x)}{\partial x} \right| = \begin{vmatrix} \frac{\partial g(x(t_1))}{\partial x(t_1)} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\partial g(x(t_r))}{\partial x(t_r)} \end{vmatrix}$$

$$\lambda \triangleq \begin{bmatrix} D_1 \\ \vdots \\ D_r \end{bmatrix}, \quad X \triangleq \begin{bmatrix} s_{X_1} \\ \vdots \\ s_{X_r} \end{bmatrix} \quad (2.48)$$

$$D_i = D(t_i) \triangleq \left. \frac{\partial x}{\partial \theta} \right|_{t=t_i}, \quad s_{X_i} = s_X(t_i) \triangleq \left. \frac{\partial x}{\partial x_0} \right|_{t=t_i}$$

$D(t)$ and $s_X(t)$ are $n \times p$ and $n \times n$ matrices, and are called sensitivity functions with respect to the parameter and initial conditions which satisfy the following differential equations,

$$\dot{D} = \left. \frac{\partial f}{\partial x} \right|_{\bar{\theta}, \bar{x}_0} D + \left. \frac{\partial f}{\partial \theta} \right|_{\bar{\theta}, \bar{x}_0}, \quad D(0) = 0 \quad (2.49)$$

$$\dot{s}_X = \left. \frac{\partial f}{\partial x} \right|_{\bar{\theta}, \bar{x}_0} \cdot s_X, \quad s_X(0) = I$$

The deviations of the estimated parameters and initial conditions from the true values θ^* and x_0^* are,

$$\theta^* = \bar{\theta} - \Delta\theta, \quad x_0^* = \bar{x}_0 - \Delta x_0 \quad (2.50)$$

y in Eqs.(2.46) and (2.47) is approximated by Tayler's Expansion and first order approximation as follows

$$y \doteq g(x) \Big|_{\bar{\theta}, \bar{x}_0} - G \cdot \lambda \cdot \Delta\theta - GX \cdot \Delta x_0 + \eta \quad (2.51)$$

Substituting Eq.(2.51) into Eqs.(2.46) and (2.47), the following

$$(\eta - G\lambda\Delta\theta - GX\Delta x_0)' W \cdot G\lambda = 0 \quad (2.52)$$

$$(\eta - G\lambda\Delta\theta - GX\Delta x_0)'W \cdot GX = 0 \quad (2.53)$$

are deduced. From Eqs. (2.52) and (2.53), $\Delta\theta$ are solved as

$$(H - KL^{-1}K^T)\Delta\theta = \lambda^T G^T W - KL^{-1}X^T G W \eta \quad (2.54)$$

where

$$\begin{aligned} H &= \lambda^T G^T W G, & K &= \lambda^T G^T W G X, \\ L &= X^T G^T W G X, \end{aligned} \quad (2.55)$$

and superscript T means transposition of a matrix.

Multiplying $\Delta\theta^T(H - KL^{-1}K^T)$ at the right hand side of Eq. (2.54), we calculated the expected value. As $E[\eta\eta^T] = M$ and we assume $E[\Delta\theta\Delta\theta^T] = P$, the following are satisfied,

$$(H - KL^{-1}K^T)P(H - KL^{-1}K^T) = (\tilde{H} - \tilde{K}L^{-1}\tilde{K}^T + \tilde{K}L^{-1}\tilde{L}L^{-1}\tilde{K}^T) \underline{\tilde{P}} \quad (2.56)$$

where

$$\begin{aligned} \tilde{H} &= \lambda^T G^T W M W G \\ \tilde{K} &= \lambda^T G^T W M W G X \\ \tilde{L} &= X^T G^T W M W G X \end{aligned} \quad (2.57)$$

Then,

$$P = (H - KL^{-1}K^T)^{-1} \tilde{P} (H - KL^{-1}K^T)^{-1} \quad (2.58)$$

are given. If we choose $W = M^{-1}$ as Eq(2.39), from the relations,

$\tilde{H} = H$, $\tilde{K} = K$ and $\tilde{L} = L$,

$$P = (H - KL^{-1}K^T)^{-1} \quad (2.59)$$

is given. If the initial value of x is given beforehand,

$$P = H^{-1} \quad (2.60)$$

Then, the variance of the deviation of parameters from true value, $\Delta\theta$, is given as P in Eq.(2.58), or Eq.(2.59), or Eq.(2.60). Similarly, the variance of the deviation of initial conditions, Δx , can be given. The confidence region is given as the following ellipsoid,

$$e : z^T P^{-1} z = 1 \quad (2.61)$$

which will be described later in this chapter.

Now if b is a unit p -vector, the linear function $b'\Delta\theta$ of $\Delta\theta$ will have a Gaussian distribution with zero mean, and its variance is given as

$$\sigma_b^2 = b' P b \quad (2.62)$$

This is clear from $E(b'\Delta\theta\Delta\theta'b) = b' P b$. Now the true parameter value θ^* is represented by using the estimated value $\bar{\theta}$ as follows,

$$\theta^* = \bar{\theta} + \Delta\theta \quad (2.63)$$

Then, from the fact that $b'(\theta^* - \bar{\theta})$ has a Gaussian distribution with the variance σ_b^2

$$|b'(\theta^* - \bar{\theta})| \leq K \cdot \sigma_b \quad (2.64)$$

is satisfied, where K depends on the chosen confidence level, for example at the 95[%] level $K=1.96$. Hence Eq.(2.64) is rewritten as follows,

$$b'\bar{\theta} - K \cdot \sigma_b \leq b'\theta^* \leq b'\bar{\theta} + K \cdot \sigma_b \quad (2.65)$$

Eq.(2.65) represents a confidence region in a specified proportion of occasions when the parameter vector $\bar{\theta}$ is projected orthogonally

upon b . If we assert that Eq.(2.65) is satisfied, then we shall be correct on a chosen level of occasion. The smaller the size of the confidence region is, the more accurately it may be said that the estimated parameter value is $\bar{\theta}$.

2-3-3 Geometrical Meaning of Parameter Fitting

(1) Preliminary mathematical knowledge

The problem of the parameter fitting can be explained skillfully by the concept of the orthogonal projection. In order to discuss this in as general a form as possible, we will argue mainly in Hilbert space but at the same time in Euclidian space. Here, mathematics which is necessary for our later discussion is given.

First, the concept of Hilbert space can be made somewhat clear by the following two definitions, but more detail is not given here, and is in many literatures, for example [2-38].

Def.-I: (inner product) Let X be a complex linear space. A rule which assigns a scalar x, y to every pair of elements $x, y \in X$ is called an inner product function if the following conditions are satisfied;

- (1) $\langle x, y \rangle = \langle y, x \rangle$ (commutative law)
- (2) $\langle x, y+z \rangle = \langle x, y \rangle + \langle x, z \rangle$ (distributive law)
- (3) $\langle \lambda \cdot x, y \rangle = \lambda \cdot \langle x, y \rangle$ for any complex λ ,
- (4) $\langle x, x \rangle \geq 0$ where $\langle x, x \rangle = 0 \rightarrow x=0$.

Def.-II: (Hilbert space) A complex linear space X is called an inner product space if a complex-valued inner product function is defined by it. A linear space X is called a Hilbert space if X is an inner product space that is complete with respect to the norm induced by the inner product.

From Def.-II, n -dim. Euclidian space in which inner product,

norm and metric are defined in the ordinary sense of Euclid is a Hilbert space. The result of a discussion of Hilbert space is applicable to a wider range of problems than one in Euclidian space. Therefore, the concept of orthogonal projection is given in Hilbert space. A definition of being orthogonal is given in Def.-III.

Def.-III: If S is any non-empty set of vectors in Hilbert space H , we say that y is orthogonal to S and write $y \perp S$ if $y \perp x$ for every x in S . The set of all vectors orthogonal to S is denoted by $S^\perp$ and is called the orthogonal complement of S .

Next, the meaning of the orthogonal projection will be put forth in the following theorem.

Theorem-I: Let L be a closed linear subspace of H . Then each x in H has a unique representation $x=y+z$ where $y \in L$ and $z \in L^\perp$. The vector y is called the projection of x onto L .

Proof: See the reference [2-38].

Furthermore, an important corollary making clear the essential meaning of the parameter fitting will be given next.

Corollary-I: Let M be a closed linear subspace of H . A unique vector $y \in M$ (the projection of x onto M) for each $x \in H$ exist such that $x-y \in M^\perp$ and y satisfies

$$\|x-y\| \leq \|x-m\| \quad \text{for all } m \in M.$$

In the Euclidian space, this corollary will be clear intuitively because it will be remembered that the minimum distance from y to the linear subspace M for $y \in \mathbb{R}^n$ is the segment of the line that is normal to M . Often, this corollary is useful not only for the problem of parameter fitting but also for many other optimal problems.

(2) Orthogonal projection

By using Corollary-I, the meaning of parameter fitting will be made clear for cases of linear and nonlinear parameter fittings.

(a) In the case of a linear parameter fitting :

Once more the problem of the linear parameter fitting is written as follows,

$$y = X \cdot \theta + \eta \quad . \quad (2.66)$$

The performance index is given as,

$$F(\theta) = (y - X\theta)' \cdot M^{-1} \cdot (y - X\theta) \quad . \quad (2.67)$$

The problem is to find the parameter value θ minimizing $F(\theta)$.

Now, a set

$$H = \{z \mid z \in R^n\} \quad (2.68)$$

is considered, and the inner product function is given as

$$\langle z^1, z^2 \rangle = (z^1)' \cdot M^{-1} \cdot (z^2) \quad , \quad (2.69)$$

where M^{-1} is defined in Eq. (2.38) symmetrical and positive definite.

The norm is defined in Eq. (2.70) as,

$$\|z\|^2 = \langle z, z \rangle = z' \cdot M^{-1} \cdot z \quad . \quad (2.70)$$

Then the set H becomes Hilbert space, for H is inner product space and complete as metric space. $F(\theta)$ given in Eq. (2.67) can be written as,

$$F(\theta) = \|y - X \cdot \theta\|^2 \quad . \quad (2.71)$$

The problem of the linear parameter fitting minimizing $F(\theta)$ in Eq.(2.67) is to find θ minimizing $\|y-X\theta\|$ in H . Now, if X is broken down into

$$X = [x_1, \dots, x_p] \quad , \quad (2.72)$$

where x_i is an n -dim. column vector for all i , then $X\theta$ is represented as,

$$X \cdot \theta = x_1 \cdot \theta_1 + \dots + x_p \cdot \theta_p \quad . \quad (2.73)$$

It is assumed that the structure of the model is correct. Then the solution of the linear parameter fitting is given as follows :

The solution $\bar{\theta}$ minimizing $F(\theta)$ given in Eq.(2.71) is given by the orthogonal projection of y onto the linear subspace S_1 which is spanned by $x_1, \dots, x_p$. Because it is seen from Eq.(2.73) that $X\theta$ is the element of the linear subspace S_1 . From Corollary-I it is evident that the orthogonal projection of y onto S_1 minimizes $\|y-X\theta\|$. That is to say, the orthogonal projection of y onto S_1 gives the solution $\bar{\theta}$ of this parameter fitting.

Furthermore, the following fact is clear.

Necessary and sufficient condition that all θ_i can be determined uniquely is that $x_1, \dots, x_p$ are linearly independent.

If $x_1, \dots, x_p$ are linearly dependent, the dimension of S_1 is less than p , and all θ_i cannot be determined uniquely.

Now, the estimated parameter value $\bar{\theta}$ is determined as follows :
Generally, we write S_1 as $X \cdot d$, where d is p -dim. vector. As the linear subspace S_1 is orthogonal to $y-X\theta$,

$$\langle X \cdot d, y - X \cdot \theta \rangle = 0 \quad , \quad (2.74)$$

then,

$$d' \hat{X} \hat{M}^{-1} \cdot (y - X \cdot \theta) = 0 \quad (2.75)$$

The equation (2.75) is valid for any vector d , and then,

$$\hat{X} \hat{M}^{-1} \cdot X \cdot \bar{\theta} = \hat{X} \hat{M}^{-1} \cdot y \quad (2.76)$$

The Eq.(2.76) coincides with Eq.(2.40) which is obtained by differentiating $F(\theta)$ with respect to θ . As seen above, the mathematical meaning of the parameter fitting is made clear by the orthogonal projection. For example, in the case of $n=2$, $p=2$, the relation of the parameter fitting is shown in Fig.2.2.

(b) In the case of nonlinear parameter fitting :

Once more the problem of nonlinear parameter fitting is written with the process equations,

$$\dot{x} = f(x, \theta, t) \quad x(0) = x_0 \quad (2.77)$$

and the observed equations,

$$y = g(x) + \eta \quad (2.78)$$

The problem is to find the parameter value θ minimizing $F(\theta)$ given as

$$F(\theta) = (y - g(x))' \cdot M^{-1} \cdot (y - g(x)) \quad (2.79)$$

Now, set N and H

$$N = \{g(x) \mid x(0) = x_0, x \in R^n, \theta \in R^p\} \quad (2.80)$$

$$H = \{z \mid z \in R^n\} \quad (2.81)$$

are considered. The inner product function and norm are defined in the same way as in the linear parameter fitting, then,

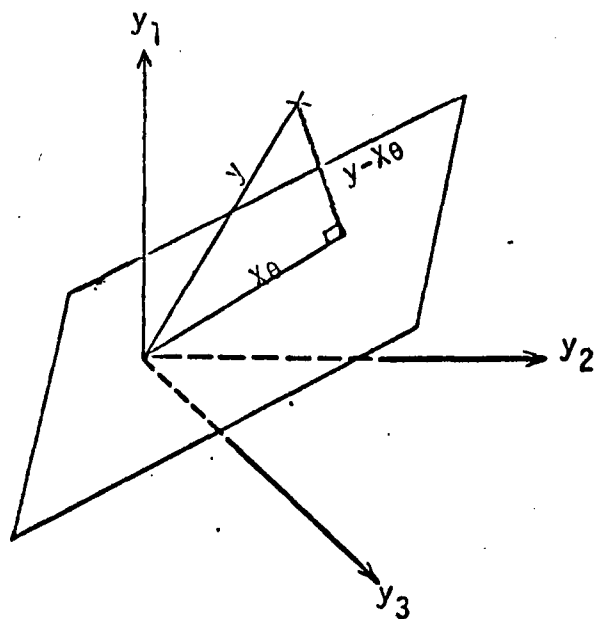


Fig. 2.2 Linear parameter fitting in the case of $n=3$, $p=2$.

$$\langle z^1, z^2 \rangle = (z^1)^T \cdot M^{-1} \cdot (z^2) \quad , \quad (2.82)$$

$$\|z\|^2 = \langle z, z \rangle = z^T \cdot M^{-1} \cdot z \quad . \quad (2.83)$$

The set H is Hilbert space, and $F(\theta)$ becomes the square of the norm from y to some point on N . Then the problem of the nonlinear parameter fitting is to find θ minimizing the norm from y to some point on N . Now N is called the solution locus. N is not a linear subspace and therefore the solution cannot be investigated directly by using Corollary-I.

In order to use Corollary-I, we will not investigate the solution directly, but adopt the basic idea of the gradient method or linearization. Now, it is assumed that the parameter value is θ . A plane tangent to the solution locus at the point corresponding to θ is considered. On this plane, θ is modified in the direction so that $F(\theta)$ is reduced to the greatest extent, where this modification is considered in the range of the tangent plane being a sufficient approximation of the solution locus.

If the modified value is $\Delta\theta$, the next thing is to do the same modification as above at $\theta + \Delta\theta$. This process continues until the minimum $F(\bar{\theta})$ is investigated. The actual calculation is shown as follows :

First, $F(\theta)$ is expanded in Taylor series with respect to θ and approximated by the first order of $\Delta\theta$, then

$$\Delta F = F(\theta + \Delta\theta) - F(\theta) = (y - g(x))^T \cdot M^{-1} \cdot G \cdot \lambda \Big|_{\theta=\theta} \cdot \Delta\theta \quad (2.84)$$

where G and λ is defined in Eq.(2.48). Next, the condition of the

step size of $\Delta\theta$

$$\Delta\theta' \cdot \omega \cdot \Delta\theta = (dp)^2 \quad (2.85)$$

is considered where ω is the weighting matrix, and $(dp)^2$ is an arbitrary constant. The modified value $\Delta\theta$ is selected to minimize the ΔF in Eq.(2.84) subject to Eq.(2.85). This is the procedure of the ordinary gradient method. The point finally arrived at, that is to say, the point given the estimated parameter value $\bar{\theta}$ is explained as below. The fact that the vector $(y-g[x])$ is orthogonal to the hyperplane S_2 spanned by $G\lambda\Delta\theta$ gives the estimated parameter value $\bar{\theta}$. From Eq.(2.82) and $\forall u \in R^p$,

$$\langle y - g(x)|_{\theta=\bar{\theta}}, G \cdot \lambda \cdot u \rangle = (y - g(x)|_{\theta=\bar{\theta}})' \cdot M^{-1} \cdot G \cdot \lambda \cdot u = 0 \quad (2.86)$$

Now, the situation where all θ_i can be determined uniquely will be considered in the same way as the linear parameter fitting.

If v_i is defined as,

$$G \cdot \lambda = [v_1, \dots, v_p] \quad (2.87)$$

where v_i is n-dim. column vector for all i , then *the necessary and sufficient condition that all θ_i can be determined uniquely is that $v_1, \dots, v_p$ are linearly independent.* Two intuitive examples that don't satisfy the above condition are shown below.

Example 2-1

We consider a parameter fitting of the rate constant in the case of a first order parallel reaction. It is assumed that the process equations are,

$$\dot{x}_1 = -(k_1 + k_2) \cdot x_1,$$

$$\begin{aligned}\dot{x}_2 &= k_1 \cdot x_1 \\ \dot{x}_3 &= k_2 \cdot x_1\end{aligned}$$

the observation done once and observed equation is,

$$y = x_1(t_1) + \eta$$

If θ is defined as,

$$\theta = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix},$$

then

$$G \cdot \lambda = (1, 0, 0) \cdot \begin{bmatrix} \frac{\partial x_1}{\partial k_1} & \frac{\partial x_1}{\partial k_2} \\ \frac{x_2}{k_1} & \frac{\partial x_2}{\partial k_2} \\ \frac{x_3}{k_1} & \frac{\partial x_3}{\partial k_2} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial k_1} & \frac{\partial x_1}{\partial k_2} \end{bmatrix} \equiv (v_1, v_2)$$

At this time $v_1 = v_2$, therefore v_1 and v_2 are linearly dependent.

Then k_1 and k_2 cannot be determined uniquely. This is natural from the intuitive fact that only x_1 is measured and that $(k_1 + k_2)$ can be determined but k_1, k_2 cannot.

Example 2-2

Now we consider the consecutive reaction. It is assumed that the process equations are

$$\begin{aligned}\dot{x}_1 &= -k_1 \cdot x_1 \\ \dot{x}_2 &= k_1 \cdot x_1 - k_2 \cdot x_2\end{aligned}$$

$$\dot{x}_3 = k_2 \cdot x_2 ,$$

the observation is done once, and the observed equation is,

$$y = x_1(t_i) + \eta .$$

If θ is defined as,

$$\theta = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix} ,$$

then

$$G \cdot \lambda = (1,0,0) \cdot \begin{bmatrix} \frac{\partial x_1}{\partial k_1} & \frac{\partial x_1}{\partial k_2} \\ \frac{\partial x_2}{\partial k_1} & \frac{\partial x_2}{\partial k_2} \\ \frac{\partial x_3}{\partial k_1} & \frac{\partial x_3}{\partial k_2} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial k_1} & \frac{\partial x_1}{\partial k_2} \end{bmatrix} \equiv (v_1, v_2) .$$

At this time, $v_2=0$ and therefore both k_1, k_2 cannot be determined uniquely.

The above two examples are clear from the intuitive fact, but we must pay attention to this condition even if it is not clear from the intuitive fact, such as in the case where all θ_i cannot be determined uniquely when $v_1, \dots, v_p$ is linearly dependent.

(3) Geometric meaning of the parameter confidence regions

(a) Geometric meaning of the parameter confidence regions :

The geometric meaning of the parameter confidence regions described previously is given here. Also the case of nonlinear para-

meter fitting is considered. It is assumed that P is symmetrical and positive definite. Then, its eigen vector is real and orthogonal. It is considered the ellipsoid given by

$$e : Z'P^{-1}Z = 1 \quad (2.88)$$

where P is defined in Eq.(2.58) and Z is the p -dim. column vector. For any unit p -vector, let h be a hyperplane normal to b and tangent to e . Then the length of the normal to h from the origin is $\sqrt{b'Pb}$. This is easily shown as follows :

The normal to e is parallel to b , then

$$P^{-1}Z = \lambda^2 b \quad (2.89)$$

From this equation,

$$Z'P^{-1}Z = \lambda^2 Z'b = 1 \quad (2.90)$$

On the otherhand, from Eq.(2.89) and Eq.(2.90),

$$Z'b = \lambda^2 b'Pb = 1/\lambda^2$$

then,

$$Z'b = \sqrt{b'Pb} \quad (2.91)$$

Furthermore $Z'b$ is the length of the normal to h from the origin.

This completes the above statement.

It will be seen from Eq.(2.62) and Eq.(2.91) that σ_b is the orthogonal projection of e onto b . In other words, if the origin is parallel and is translated to the top of the estimated parameter vector $\bar{\theta}$, the standard deviation of the orthogonal projection $b'\theta$ of θ upon b of the ellipsoid e , for example, when $n=3$, $p=2$ is considered in Fig.2.3 and Fig.2.4. Now let θ^* be the true parameter

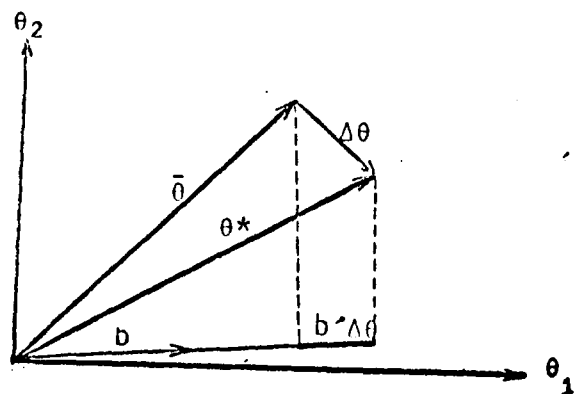


Fig. 2.3 Projection of $\Delta\theta$ upon b .

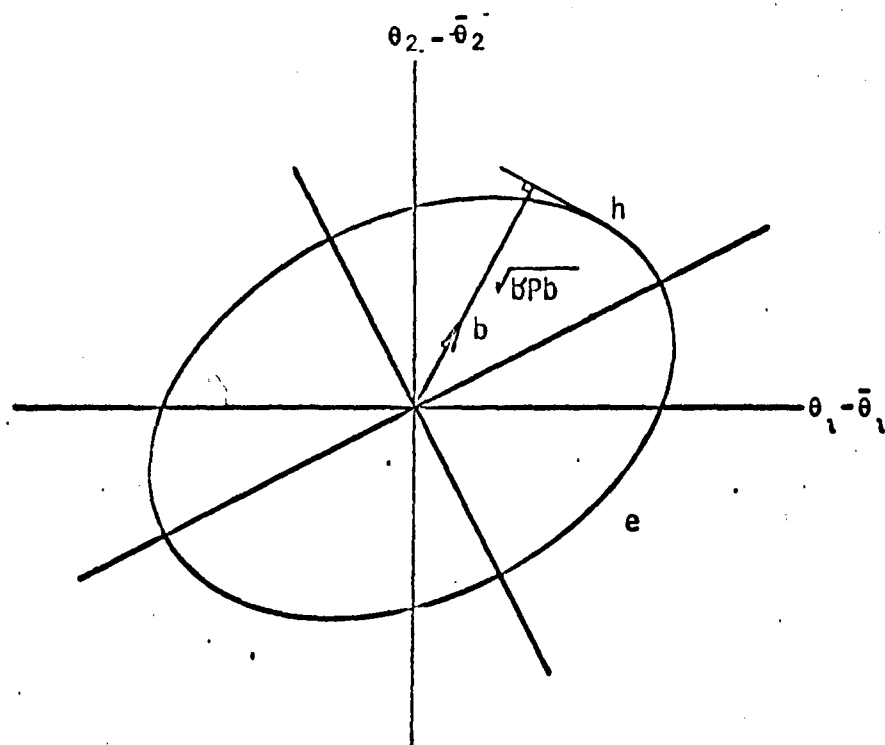


Fig. 2.4 Confidence interval of $b'\Delta\theta$.

value, and then $b'\Delta\theta$ is the orthogonal projection of $(\theta - \bar{\theta})$ upon b . When the origin is parallel and translated to $\bar{\theta}$, the relation of σ_b to e is illustrated in Fig.2-4.

The figure and size of e gives information about the parameter confidence regions.

Next, we consider the figure and the size of e .

Let λ be an eigen value of P and $\circ\lambda$ be a eigen value of P^{-1} .

$$\circ\lambda = \frac{1}{\lambda} \quad (2.92)$$

is satisfied. Let $e_1, \dots, e_p$ be the eigen vector of P^{-1} and different from each other, and let T be the orthogonal matrix constructed by $e_1, \dots, e_p$ as follows,

$$T = [e_1, \dots, e_p] \quad (2.93)$$

If P^{-1} is orthogonally transformed by T ,

$$T^{-1} \cdot P^{-1} \cdot T = T \cdot P^{-1} \cdot T = \begin{bmatrix} \circ\lambda_1 & & 0 \\ & \ddots & \\ 0 & & \circ\lambda_p \end{bmatrix} \quad (2.94)$$

Now in the following transformation

$$Z = T \cdot v \quad (2.95)$$

is substituted into Eq.(2.88), then

$$v' \begin{bmatrix} \circ\lambda_1 & & \\ & \ddots & \\ & & \circ\lambda_p \end{bmatrix} \cdot v = 1 \quad (2.96)$$

where v is p -dim. column vector.

The volume of the ellipsoid given in Eq.(2.96) is proportional to $\frac{1}{\sqrt{\prod_{i=1}^p \circ\lambda_i}}$. Then, the volume of the ellipsoid e given in Eq.(2.88) is

proportional to $1/\prod_{i=1}^p \lambda_i$, for the volume is not changed by the orthogonal transformation. Paying attention to

$$\frac{1}{\prod_{i=1}^p \lambda_i} = \prod_{i=1}^p \lambda_i^{-1} = |P|^{-1}, \quad (2.97)$$

it is seen that the volume of e is proportional to $|P|$ which denotes the determinant of P . Accordingly, the smaller $|P|$ is, the smaller the volume of the ellipsoid e is. If we don't take into account the figure of e , it may be said that the accuracy of the parameter fitting is proportional to the volume of e ; in other words, $|P|$. Then $|P|$ is useful for the judgement of the accuracy of the parameter fitting. This fact is applied in Chapter 3 to the design of the experiment.

Now once more notice Eq.(2.94). The figure of e will be approximated without writing the ellipsoid. For example the semidiameter of e is $1/\sqrt{\lambda_i}$. If the longest semidiameter is R_1 and the shortest semidiameter is R_2 , then

$$R_1 = \max_i \left\{ \frac{1}{\sqrt{\lambda_i}} \right\} = \max_i \{ \sqrt{\lambda_i^{-1}} \}, \quad (2.98)$$

$$R_2 = \min_i \left\{ \frac{1}{\sqrt{\lambda_i}} \right\} = \min_i \{ \sqrt{\lambda_i^{-1}} \}. \quad (2.99)$$

As shown above, all the information on the parameter confidence regions are contained in the eigen-values and eigen-vectors of P .

Example 2-3

We now consider the case where $p=2$. It is assumed that P is given as follows,

$$P = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix} \quad \text{and} \quad P^{-1} = \begin{bmatrix} 3/5 & -1/5 \\ -1/5 & 2/5 \end{bmatrix} .$$

The eigen-values of P^{-1} are,

$$\lambda_1 = \frac{5 + \sqrt{5}}{10} \quad \text{and} \quad \lambda_2 = \frac{5 - \sqrt{5}}{10} .$$

The unit eigen-vectors of P^{-1} are respectively,

$$e_1 = \begin{bmatrix} \frac{2}{\sqrt{10-2\sqrt{5}}} \\ \frac{1-\sqrt{5}}{\sqrt{10-2\sqrt{5}}} \end{bmatrix} , \quad e_2 = \begin{bmatrix} \frac{2}{\sqrt{10+2\sqrt{5}}} \\ \frac{1+\sqrt{5}}{\sqrt{10+2\sqrt{5}}} \end{bmatrix} .$$

Now the ellipsoid e

$$e : Z \cdot P^{-1} \cdot Z = 1$$

is orthogonally transformed by T in Eq.(2.93) and the ellipsoid e is transformed as,

$$\frac{(v_1)^2}{\frac{10}{5+\sqrt{5}}} + \frac{(v_2)^2}{\frac{10}{5-\sqrt{5}}} = 1 .$$

The volume of e is

$$\text{vol. of } e = \pi \cdot \left[\frac{10}{5+\sqrt{5}} \cdot \frac{10}{5-\sqrt{5}} \right]^{0.5} = \pi \cdot (|P|)^{0.5} = \sqrt{5} \cdot \pi .$$

(b) Sample space and parameter space

Now we consider the case of nonlinear parameter fitting, but the following discussion is the same as for the case of linear parameter fitting if $G\lambda = X$. As shown previously, it is considered that the orthogonal projection of y onto p -dim. hyperplane S_2 spanned by $v_1, \dots, v_p$ gives the estimated parameter value $\bar{\theta}$, where $y \in H$. This orthogonal projection is given as $G\lambda\bar{\theta}$. $G\lambda\bar{\theta}$ is defined as,

$$G\lambda\bar{\theta} = \theta_1 \cdot v_1 + \dots + \theta_p \cdot v_p \equiv V \cdot \bar{\theta} \quad (2.100)$$

H is called sample space.

Next draw a line from y to S_2 and let the intersection trace out where the length from y to the intersection of this line is identical. If the vector with its top on this trace is Vu (naturally $Vu \in S_2$), then

$$|V \cdot (\bar{\theta} - u)|^2 = |y - V \cdot u|^2 - |y - V \cdot \bar{\theta}|^2 = \text{constant} \equiv K \quad (2.101)$$

because

$$V \cdot (\bar{\theta} - u) \perp (y - V \cdot u) \quad (2.102)$$

From the equation (2.101), this trace is p -dim. hypersphere on S_2 . We must pay attention to the fact that the basis of this hypersphere is orthogonal basis taken in H . The origin being parallel and translated to $V\bar{\theta}$,

$$(V \cdot u) : M^{-1} \cdot V \cdot u = K \quad (2.103)$$

is satisfied. The p -dim. hyperplane S_2 spanned by $v_1, \dots, v_p$ (as the basis) is called the parameter space. That is to say, in the parameter space the basis of S_2 defined in H is taken as $v_1, \dots, v_p$.

From Eq. (2.103),

$$u' \hat{V} \hat{M}^{-1} \cdot V \cdot u = u' \hat{\lambda}' \cdot G \cdot M^{-1} \cdot G \cdot \lambda \cdot u = u' \hat{P}^{-1} \cdot u = K \quad (2.104)$$

This equation corresponds to the ellipsoid e given in Eq. (2.88). As shown above, the parameter confidence region in the parameter space is the hypersphere on S_2 defined in sample space H . This shows the relationship between the sample space and parameter space.

2-4. PARAMETER ESTIMATION IN ORDINARY DIFFERENTIAL EQUATIONS BY D.F.P.

2-4-1 Computational Method

We consider the following parameter estimation problem :

The system equation is

$$\dot{x} = f(x, P) , \quad x(0) = x_0 \quad (2.105)$$

The observation at $t=t_r$ is given by

$$y_r = g[x(t_r, P^*)] + \eta_r , \quad r=0, \dots, R \quad (2.106)$$

where x is n -dim. state vector, P is p -dim. parameter vector, y_r is m -dim. output or observation vector and η_r is m -dim. error vector.

Parameters P are estimated so as to minimize $F(P)$ in Eq.(2.107),

$$F(P) = \sum_{r=1}^R (y_r - g[x(t_r, P)])^T W_r (y_r - g[x(t_r, P)]) \quad (2.107)$$

This parameter estimation problem can be reduced to the parametric optimization problem which is to find the constant parameter so as to minimize some objective function under certain constraints. Then, various so-called optimization techniques may be used, in which case we must solve two point boundary value problem generally. To solve these formulae, however, may not be so easy because the dimension of the variables is very large. Then, searching methods by iterative calculation^{[2-38]~[2-42]}, such as the direct search method, various gradient methods, Marquardt method, and quasi-linearization method may be preferable in solving the parameter estimation problem. This has been described in Chapter 1. Parameter estimation

by the steepest descent method is described briefly in 1-1-4 and in more detailed in Chapter 7. Here we will formulate this parameter estimation problem by the conjugate gradient method^{[2-43]~[2-45]}. Davidon Fletcher Powell method (termed by D.F.P. hereafter)^[2-43] is used for the conjugate gradient method.

2-4-2 Parameter Estimation by D.F.P.

We assume that the initial condition x_0 must be estimated.

Calculation procedure are given in the following steps :

- i) Assume that i-th value of P and x_0 are P^i and x_0^i . Calculate $x(t)$ and $\partial f/\partial x$, $\partial f/\partial P$ based on P^i and x_0^i .
- ii) Determine the direction of conjugate gradient d,

$$\left. \frac{\partial F}{\partial P} \right|_i = -2 \sum_{r=0}^R (y_r - g[x(t_r, P)])^T W_r \cdot \frac{\partial g}{\partial x} \cdot \frac{\partial x}{\partial P} \bigg|_{t=t_r} \quad (2.108)$$

$$\left. \frac{\partial F}{\partial x_0} \right|_i = -2 \sum_{r=0}^R (y_r - g[x(t_r, P)])^T W_r \cdot \frac{\partial g}{\partial x} \cdot \frac{\partial x}{\partial x_0} \bigg|_{t=t_r} \quad (2.109)$$

where $\left. \frac{\partial x}{\partial P} \right|_{t=t_r}$ and $\left. \frac{\partial x}{\partial x_0} \right|_{t=t_r}$ are sensitivity coefficients

which satisfy the following equations. When we assume

$\left. \frac{\partial x}{\partial P} \right|_{t=t_r} \triangleq D(t_r)$, $\left. \frac{\partial x}{\partial x_0} \right|_{t=t_r} \triangleq X(t_r)$, then D(t) and X(t) satisfy

the following equations,

$$\frac{dD}{dt} = \frac{\partial f}{\partial x} D + \frac{\partial f}{\partial P} \quad , \quad D(t_0)=0 \quad (2.110)$$

$$\frac{dX}{dt} = \frac{\partial f}{\partial x} X \quad , \quad X(t_0)=I \quad (2.111)$$

where $\partial f/\partial P$, $\partial f/\partial x$, $\partial g/\partial x$ are evaluated at P^i and x_0^i . Then $\partial F/\partial P$ and $\partial F/\partial x_0$ can be calculated. The direction of the conjugate gradient, d , is given by,

$$d_i = -H_{i-1} \cdot g_i \quad (2.112)$$

where,

$$g_i = \left[\frac{\partial F}{\partial P} \Big|_i, \frac{\partial F}{\partial x_0} \Big|_i \right] \quad (2.113)$$

H_i in Eq.(2.112) is given in step iv) where $H_0 = I$.

iii) Searching on a direction of the conjugate gradient;

If we define

$$\theta = \begin{bmatrix} P \\ x_0 \end{bmatrix} \quad (2.114)$$

we search for the minimum of $F(\theta)$ on a direction of the conjugate gradient. That is, we determine λ_i which minimize $F(\theta_i + \lambda_i d_i)$ by some direct search method. We use here a Fibonacci search. Then, $(i+1)$ th estimated values of parameters are given as,

$$\theta_{i+1} = \theta_i + \lambda_i d_i \quad (2.115)$$

Next calculate g_{i+1} by Eq.(2.113).

iv) Calculation of H_i ;

H_i is given as

$$H_i = H_{i-1} + \lambda_i \frac{d_i d_i^T}{g_i^T H_{i-1} g_i} - \frac{H_{i-1} y_i y_i^T H_{i-1}}{y_i^T H_{i-1} y_i} \quad (2.116)$$

where $y_i = g_{i+1} - g_i$

v) θ_{i+1} is taken as (i+1)th iteration. Then go back to step ii), and continue the calculation so as to satisfy the convergence criteria.

vi) Calculate the confidence region or confidence interval by using Eq. (2.58).

More detailed computer program is given in the literature^[2-46].

2-4-3 Example

We consider the estimation of reaction rate constants of the system shown in Fig.2.5. All reaction paths are assumed to be of the first order. The experimental data from batch experiments are given in Table 2.2. The number of parameters to be estimated is nine. These parameters are estimated by the D.F.P. described above. The results are shown in Table 2.3 which shows the estimated parameter value and 95[%] confidence interval at $b_i=1$, $b_j=0$ ($i \neq j$) as calculated in Eq.(2.65). The calculated value of A_i based on these estimated values of parameter are also shown in Fig.2.6.

When the number of parameters to be estimated become larger, the calculation of parameter estimation may generally be difficult. Parameter estimation by the D.F.P., however, may be applicable as shown from this example, if the number of parameters is large.

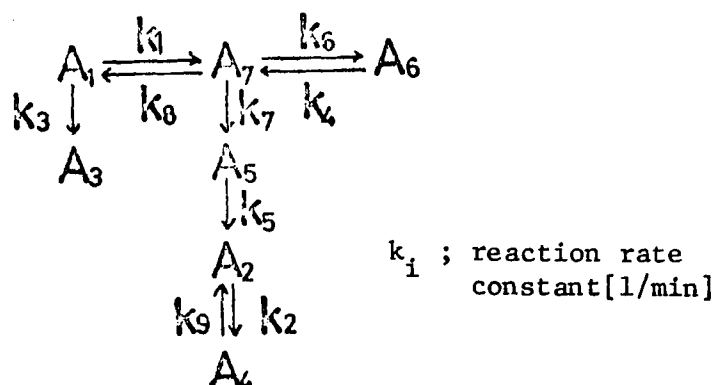


Fig. 2.5 Complex reaction system

Table 2.2 Observed data.

Time Comp. (min)	0	15	30	45	60	90	120	150	180
A ₁	1.0	0.649	0.412	0.284	0.175	0.159	0.096	0.049	0.059
A ₂	0.0	0.048	0.021	0.046	0.00	0.033	0.064	0.031	0.025
A ₃	0.0	0.042	0.103	0.110	0.181	0.149	0.199	0.157	0.164
A ₄	0.0	0.048	0.0	0.0	0.0	0.0	0.0	0.0	0.033
A ₅	0.0	0.0	0.152	0.082	0.116	0.208	0.209	0.166	0.243
A ₆	0.0	0.0	0.123	0.274	0.300	0.338	0.448	0.450	0.476
A ₇	0.0	0.201	0.145	0.110	0.205	0.081	0.045	0.077	0.017

Table 2.3 Estimated parameter.

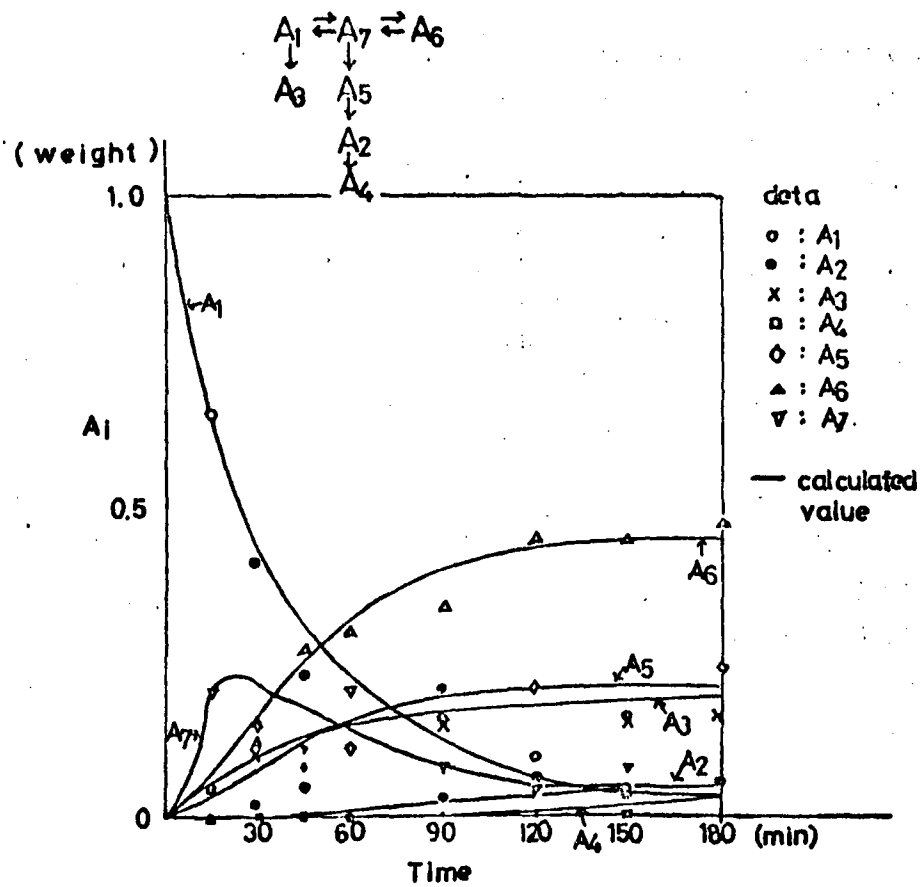
$$\begin{aligned}
 0.0258 &\leq k_1 = 0.0282 \leq 0.0806 \\
 -0.0006 &\leq k_2 = 0.0076 \leq 0.0158 \\
 0.0047 &\leq k_3 = 0.0049 \leq 0.0051 \\
 0.0021 &\leq k_4 = 0.0025 \leq 0.0028 \\
 0.0028 &\leq k_5 = 0.0029 \leq 0.0035 \\
 0.0307 &\leq k_6 = 0.0322 \leq 0.0837 \\
 0.0156 &\leq k_7 = 0.0160 \leq 0.0164 \\
 0.0175 &\leq k_8 = 0.0186 \leq 0.0197
 \end{aligned}$$


Fig. 2.6 Result of parameter estimation.

NOMENCLATURE

b	; true parameter
D	; sensitivity function of x with respect to θ
e	; error of observed and calculated value
f	; function of state variables
g	; observing function
M_i	; covariance matrix of random error
$p(z)$	; probability
$p(z b)$	; conditional probability
$R(\beta)$	; average risk
T	; orthogonal matrix
u	; input
w	; noiseless output
W_i	; weighting matrix
x	; state vector
y	; output variable
z	; system output
θ	; parameter vector
$\Delta\theta$	; small deviation of parameter
σ_b^2	; variance
η	; error vector

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CHAPTER 3

DETERMINATION OF EXPERIMENTAL CONDITIONS TAKING INTO ACCOUNT THE EFFECT OF PARAMETER ACCURACY ON SYSTEM DESIGN

3-1. INTRODUCTORY REMARKS

In general, many experiments and observations must be performed so that the values of parameters in a mathematical model of a system can be obtained as accurately as possible. For complex system, values of parameters are roughly estimated in haste, and then, through continuing experiments and observations, consecutive modifications of sampling methods or experimental conditions must be carried out to obtain more accurate values. This chapter concerns a method for the modification of experimental conditions.

The errors of estimated parameter values may be described by an ellipsoid in the parameter space called "the parameter confidence region". The shape and size of the ellipsoid depend on the experimental conditions and parameter sensitivities of state variables. From this point of view, the policies minimizing the volume of the ellipsoid^[3-1] and those spherizing the ellipsoid^[3-2] have been proposed, and other considerations^{[3-3]~[3-6]} have been taken into

account. In these proposed methods, only the shape and size of the ellipsoid have been discussed. For actual system synthesis, however, a mathematical model with estimated parameters is necessary, and the values of these parameters must be obtained by experiments and observations for the above mathematical model. Therefore, the effect of errors of estimated parameter values on system synthesis is an important problem that can not be solved only by the size and shape of the parameter confidence region. For example, in a process design, all parameters in a mathematical model used for the design may not be estimated with the same accuracy, but parameters must be estimated so that the influence of errors in them on process design is minimized^[3-7].

3-2. PARAMETER CONFIDENCE REGION

The concept of parameter confidence region is mathematically stated as follows: The state equations are given by

$$\dot{x} = f(x, a^0, \theta) \quad (3.1)$$

where x , a^0 and θ represent the n -column-vector of state variables, l -column-vector of experimental conditions such as temperature or pressure through the experiments and p -column-vector of parameters to be estimated, respectively. Observations y_r at time t_r can be expressed by

$$y_r = g[x(t_r, a^0, \theta^*)] + \eta_r \quad r=0, \dots, R \quad (3.2)$$

where y_r is the m -column-vector and η_r is the m -column error vector of the observations. Vector θ^* presents the true value of the parameters. It is assumed that η_r has a Gaussian distribution with zero mean and covariance M_r , and that η_i and η_j are statistically independent ($i \neq j$).

Hereafter, experimental conditions are assumed to contain a^0 and sampling time t_r ($r=0, 1, \dots, R$); These conditions are represented by vector a , to distinguish a from a^0 . Moreover, experimental conditions a are assumed to be fixed at the values designated beforehand. That is to say, the values of parameters are estimated from the results of experiments which are performed under fixed experimental conditions. Then, the optimal conditions are determined by various methods, described later, based on the estimated parameter $\bar{\theta}$. Next, experiments are performed according to optimal experimental conditions. This procedure will be continued until estimated parameters are suitably accurate.

Least-square estimation of parameters with weighting factor M_r^{-1} is used to find the parameter values which minimize $F(\theta)$ in the following Eq.(3.3) subject to Eq.(3.1) and Eq.(3.2),

$$F(\theta) = \sum_{r=0}^R (y_r - g[x(t_r, a^0, \theta)])' M_r^{-1} (y_r - g[x(t_r, a^0, \theta)]) \quad (3.3)$$

where superscript ' and -1 represent the transpose vector or matrix and inverse matrix, respectively. The parameter confidence region of the estimated parameter $\bar{\theta}$ is described by an ellipsoid in Eq.(3.4) in the p -dimensional parameter space,

$$z' P^{-1} z = 1 \quad (3.4)$$

where P represents the covariance of $\delta\theta$, the error of $\bar{\theta}$ deviated from true parameter value θ^* , and is given by^[3-8]

$$P \triangleq \text{Expectation}[\delta\theta \cdot \delta\theta'] = [H - N \cdot L^{-1} \cdot N']^{-1} \quad (3.5)$$

where,

$$\begin{aligned} H &= \sum_{r=0}^R D_r' G_r' M_r^{-1} G_r D_r \\ N &= \sum_{r=0}^R D_r' G_r' M_r^{-1} G_r X_r \\ L &= \sum_{r=0}^R X_r' G_r' M_r^{-1} G_r X_r \end{aligned}$$

In Eq.(3.5), D_r and X_r represent the sensitivity coefficients at time t_r of state variables due to the parameter deviations and initial conditions, respectively, and which satisfy the following sensitivity equations,

$$\begin{aligned} \dot{D} &= \frac{\partial f}{\partial x} D + \frac{\partial f}{\partial \theta} \quad , \quad D(t_0)=0, \quad D_r \triangleq D(t_r) \\ \dot{X} &= \frac{\partial f}{\partial x} X \quad , \quad X(t_0)=I \text{ (unit matrix)}, \quad X_r \triangleq X(t_r) \end{aligned} \quad (3.6)$$

where,

$$D = \begin{vmatrix} \frac{\partial x_1}{\partial \theta_1} & \dots & \frac{\partial x_1}{\partial \theta_p} \\ \vdots & & \vdots \\ \frac{\partial x_n}{\partial \theta_1} & \dots & \frac{\partial x_n}{\partial \theta_p} \end{vmatrix}$$

$$X = \begin{vmatrix} \frac{\partial x_1}{\partial x_1(t_0)} & \dots & \frac{\partial x_1}{\partial x_n(t_0)} \\ \vdots & & \vdots \\ \frac{\partial x_n}{\partial x_1(t_0)} & \dots & \frac{\partial x_n}{\partial x_n(t_0)} \end{vmatrix}$$

G_r is given by

$$G_r = \left| \frac{\partial g[x(t_r, \alpha^0, \theta)]}{\partial x(t_r, \alpha^0, \theta)} \right| \quad (3.7)$$

where partial differential terms in Eq.(3.6) and Eq.(3.7) are calculated based on the nominal parameter value $\bar{\theta}$. Furthermore, confidence intervals are given by the form of the projection of the ellipsoid to a p-dimensional unit vector b as follows,

$$|b' \delta \theta| \leq K \cdot \sigma_b, \quad \sigma_b^2 = b' P \cdot b \quad (3.8)$$

where K is a constant depending on the chosen confidence level.

For example, at 95[%] level $K=1.96$. It should be noticed that the parameter confidence region and interval are given by Eq.(3.4) and Eq.(3.8), which depend on P^{-1} .

3-3. DETERMINATION OF EXPERIMENTAL CONDITIONS BASED ONLY ON THE PARAMETER CONFIDENCE REGION

Optimal experimental conditions minimizing the volume of ellipsoid : If the overall accuracy of the estimated parameters can be defined by the volume of the parameter confidence region, the optimal experimental conditions by which most accurate values of parameters will be estimated can be given the method minimizing the volume of the ellipsoid shown by Eq.(3.4). The smaller the volume of the ellipsoid, the higher the overall accuracy of the estimated parameters becomes. The symmetric matrix P^{-1} is diagonalized by a suitable orthogonal matrix T as follows,

$$T'P^{-1}T = \begin{vmatrix} \lambda_1 & & & 0 \\ & \ddots & & \\ & & \lambda_i & \\ 0 & & & \ddots & \\ & & & & \lambda_p \end{vmatrix} \quad (3.9)$$

where λ_i is an eigen value of P^{-1} . Then, each semidiameter of the ellipsoid represented by Eq.(3.4) is given by $1/\sqrt{\lambda_i}$. Since the volume of the ellipsoid corresponds to the multiplication of each semidiameter, $1/\prod_{i=1}^P \sqrt{\lambda_i}$, and $\prod_{i=1}^P \sqrt{\lambda_i}$ is equal to the determinant of P^{-1} , then the optimal experimental conditions α which contain sampling time and α° to minimize the volume, can be attained by satisfying the following condition :

$$\underset{\alpha}{\text{Max}}\{\det(P^{-1})\} \Big|_{\theta=\bar{\theta}} \quad (3.10)$$

Optimal experimental conditions spherizing the ellipsoid :

The experimental conditions minimizing the volume of ellipsoid may be attained based on a measure of the overall accuracy of estimated parameters, but it does not take into account of the accuracy of each parameter. In so far as it is subject to Eq.(3.10), it may be that some parameters are estimated more accurately than others. Therefore, in some cases, it may be desirable that all parameters in a mathematical model have the same degree of accuracy for the purpose of system design. It is rational for a comparison of error of each estimated parameter to use the relative value of each error. That is, P^{-1} must be weighted by Θ , defined by

$$\Theta = \begin{vmatrix} |\theta_1| & & 0 \\ & \ddots & \\ 0 & & |\theta_p| \end{vmatrix} \quad (3.11)$$

Defining

$$P_0^{-1} = \Theta' P^{-1} \Theta \quad (3.12)$$

P_0^{-1} should be used in place of P^{-1} in Eq.(3.4). Estimating each parameter value with the same accuracy means that each parameter has the same estimated relative error. To do this the semidiameters of ellipsoid caused by P_0^{-1} must be equal to each other. Equalizing the semidiameters of the ellipsoid, that is, spherizing the ellipsoid, minimizes the standard deviation of $1/\sqrt{\lambda_i^0}$. The optimal experimental condition spherizing the ellipsoid is attained by the condition,

$$\min_{\theta} \left\{ \sum_{i=1}^p \left(\frac{1}{\lambda_i^{\theta}} \right)^2 - \frac{1}{p} \left(\sum_{i=1}^p \frac{1}{\sqrt{\lambda_i^{\theta}}} \right)^2 \right\} \quad (3.13)$$

where λ_i^{θ} is an eigen value of P_0^{-1} .

3-4. OPTIMAL EXPERIMENTAL CONDITIONS TAKING INTO ACCOUNT THE EFFECT ON PROCESS DESIGN

In the case of process design, generally, there is some information about the main requirements of the process to be designed. Therefore, it is rational to select the experimental conditions so that the influence of parameter errors on requirements of process design becomes as small as possible. Requirements of process design are generally described by an objective function of process design and output values to be fixed. Then, it is very important to know the effects of parameter errors on these values. Now let's consider the following problem of process design. It is assumed that the process equations are represented by

$$\dot{x} = h(x, \theta, u, t) \quad , \quad x(t_0) = x_0 \quad (3.14)$$

The optimal process design problem is to choose design variables u which minimize the value of the objective function shown by,

$$J = \int_{t_0}^{t_f} q(x, \theta, u, t) \cdot dt \quad (3.15)$$

Information about the influence of parameter deviation on this process design should be used for determining experimental conditions. The sort of information to be used depends on the kind of practical design problem.

Application of parameter sensitivity to objective function : Process design problems subject to Eq.(3.14) and Eq.(3.15) are solved by using estimated parameter value $\bar{\theta}$. Since it is desirable that the objective function not be affected by parameter error even if $\bar{\theta}$ is

not the true value, experimental conditions α should be selected so as to minimize the deviation of the objective function due to parameter deviation. One of the methods for the above policy is to select α subject to Eq.(3.16).

$$\begin{aligned} \text{Min}_{\alpha} \{ \text{Max}_{\delta\theta} (\delta J = \sum_{i=1}^p \frac{\partial J}{\partial \theta_i} \delta \theta_i) \} \Big|_{\theta=\bar{\theta}} \end{aligned} \quad (3.16)$$

subject to Eq.(3.8)

The method under this condition means to choose α minimizing the maximum deviation of the objective function due to parameter deviation under a certain confidence level.

Another method is to modify P^{-1} in Eq.(3.4) by weighting factor $\partial J / \partial \theta_i$ and using Eq.(3.13). That is,

$$P_1^{-1} = \begin{vmatrix} \frac{1}{\left| \frac{\partial J}{\partial \theta_1} \right|} & & 0 \\ & \ddots & \\ 0 & & \frac{1}{\left| \frac{\partial J}{\partial \theta_p} \right|} \end{vmatrix} \cdot P^{-1} \cdot \begin{vmatrix} \frac{1}{\left| \frac{\partial J}{\partial \theta_1} \right|} & & 0 \\ & \ddots & \\ 0 & & \frac{1}{\left| \frac{\partial J}{\partial \theta_p} \right|} \end{vmatrix} \quad (3.17)$$

$$\text{Min}_{\alpha} \left\{ \sum_{i=1}^p \left(\frac{1}{\lambda_i^1} \right)^2 - \frac{1}{p} \left(\sum_{i=1}^p \frac{1}{\sqrt{\lambda_i^1}} \right)^2 \right\} \Big|_{\theta=\bar{\theta}} \quad (3.18)$$

where λ_i^1 is an eigen value of P_1^{-1} . This policy means there is a need to estimate some of the parameters more accurately so that the deviation of these parameters affects the objective function J as little as possible.

Application of parameter sensitivity to output values to be fixed:
In order to decrease the effect of parameter deviation on the output variable and to increase the accuracy of parameter identification,

the experimental conditions must be chosen to minimize change of the output variable due to parameter change. One of the methods is to use Eq.(3.18) with the weighted P^{-1} similar to Eq.(3.17).

Another method is to search first for the parameters which affect the output variables strongly, and then to select the experimental conditions α which minimize the volume of the confidence region of only these parameters. If $\theta_1, \dots, \theta_s$ ($1 \leq i \leq s \leq p$) strongly affect the output variables, α is chosen to satisfy the condition,

$$\text{Max}_{\alpha} \left\{ \det \begin{vmatrix} -1 & \dots & -1 \\ p_{i1}^{-1} & \dots & p_{is}^{-1} \\ \vdots & & \vdots \\ -1 & \dots & -1 \\ p_{s1}^{-1} & \dots & p_{ss}^{-1} \end{vmatrix} \right\} \Big|_{\theta=\bar{\theta}} \quad (3.19)$$

where p_{ij}^{-1} is the (i,j) element of P^{-1} .

The selection of these methods may depend on the case in question.

3-5. NUMERICAL EXAMPLE

In this section the thermal decomposition reaction of the wet-air oxidation process of sludge shown in Fig.3.1 is considered^[3-9]. It is assumed that the state equations of the reaction are given by

$$\frac{dx}{d\tau} = \begin{bmatrix} -(k_1+k_2), & 0 \\ k_1-k_4, & -(k_3+k_4) \end{bmatrix} \cdot x + \begin{bmatrix} 0, & 0 \\ k_4, & k_4 \end{bmatrix} x_0 \quad (3.20)$$

where,

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad x_0 = \begin{bmatrix} x_1^0 \\ x_2^0 \end{bmatrix}$$

and x_0 is initial state. Problem is to identify the values of k_i from batch reaction experiments. In Eq.(3.20), τ , k_i and x are dimensionless time, dimensionless rate constant and dimensionless concentration, respectively. Representing real time, real rate constant and real concentration by t , $\bar{k}_i$ and $\bar{x}_i$, τ , k_i and x_i are given as

$$\tau = \left(\sum_{i=1}^4 \bar{k}_i \right) t, \quad k_i = \frac{\bar{k}_i}{\sum_{i=1}^4 \bar{k}_i}, \quad x_i = \frac{\bar{x}_i}{\sum_{i=1}^4 \bar{x}_i^0} \quad (3.21)$$

It is assumed that observations y_r are given by

$$y_r = x_r + \eta_r, \quad r = 0, \dots, 5 \quad (3.22)$$

and the observation of initial state x_0 is also subjected to Eq.(3.22).

These parameters identified are used for the purpose of optimum design problem to minimize the following objective function J by choosing a volume V of a completely mixed tank reactor in

steady state,

$$J = V - \alpha \bar{x}_2 - \beta \bar{x}_3 + \gamma \bar{x}_1 \quad (3.23)$$

where α , β and γ are constants given in Table 3.1. The other values used in this example are also given in Table 3.1. The optimal solution of this design problem by using the nominal value of parameters is obtained as follows : $V = 4 \times 10^3 [10^3 \text{cm}^3]$, $J_{\text{opt}} = 7.8 \times 10^2 [10^3 \text{cm}^3]$, $\bar{x}_{1,t_f} = 1.10 [\text{g/kg}]$, $\bar{x}_{2,t_f} = 5.86 [\text{g/kg}]$, $\bar{x}_{3,t_f} = 17.04 [\text{g/kg}]$. In this example, only five sampling times $\tau_i (i=1,2,\dots,5)$ are considered as experimental condition α .

Now let's determine these optimal five sampling times subjected to the various methods stated above. In numerical calculation, the confidence interval for δk_1 is found by putting $b_1=1$; $b_j=0$, $j \neq 1$ where $\delta \theta' = [\delta k_1, \dots, \delta k_4]$ and $b' = [b_1, \dots, b_4]$ in Eq.(3.8). The confidence level is chosen so as to be 95[%] reliable and $K=1.96$.

Six cases are considered as follows : (1) One which is subject to Eq.(3.10), (2) Subject to Eq.(3.13), (3) Subject to Eq.(3.16), (4) Subject to Eq.(3.18), (5) Subject to Eq.(3.19), and (6) arbitrary selection of sampling time for comparison with case(1)~case(5). The optimal sampling times in each case and the perturbation of the objective function and output variables in the worst case at 95[%] confidence level are shown in Table 3.2. In Table 3.2, $\det(P^{-1})$, which corresponds to the reciprocal of the volume of the ellipsoid, is also shown on the basis of case(1). The comparison of δJ or $\delta \bar{x}_{1,t_f}$ in each case shows that the influence of the error of estimated parameters on the objective function and system output variables is not small even if the volume of the ellipsoid is the

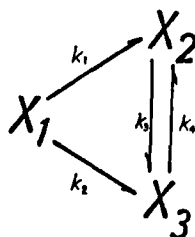


Fig. 3.1 Reaction model of thermal decomposition.

Table 3.1 Values used in example.

Batch type experiment	Design problem
$k_1 = 0.40, k_2 = 0.21$	$k_1 = 0.237, k_2 = 0.122$
$k_3 = 0.31, k_4 = 0.08$	$k_3 = 0.184, k_4 = 0.045 [1/\text{min}]$
$x_1^0 = 0.67,$	input conc.
$x_2^0 = 0.33,$	$\bar{x}_1^0 = 16, \bar{x}_2^0 = 8, \bar{x}_3^0 = 0 [g/kg]$
$x_3^0 = 0.0$	density of sludge $1.0 [g/cm^3]$
	mass flowrate $100 [kg/min]$
	$\alpha = 100 [kg \cdot 10^3 cm^3/g]$
$M_r = 1 \cdot \sigma^2, r = 0, \dots, 5$	$\beta = 400 [kg \cdot 10^3 cm^3/g]$
	$r = 3800 [kg \cdot 10^3 cm^3/g]$

Table 3.2 Comparison of optimal experimental conditions by various methods.

Method	Optimal sampling time τ	$\det [P^{-1}]$	95% confidence interval $\delta \bar{k}_i$ where $b_i=1$, $b_j=0$	Perturbation of J in the worst case on 95% confi. level ($\times 10^3$)	Perturbation of $\bar{X}_{i,f}$ in the worst case on 95% confi. level
Case (1) subject to Eq.(10)	0.2, 1.7, 2.0 5.5, 46.0	100	$\delta \bar{k}_1 = \pm 4.24\sigma$ $\delta \bar{k}_2 = \pm 4.20\sigma$ $\delta \bar{k}_3 = \pm 2.23\sigma$ $\delta \bar{k}_4 = \pm 0.90\sigma$	$\delta J = +1304\sigma$	$ \delta \bar{x}_1 _{i,f} = 23.0\sigma$ $ \delta \bar{x}_2 _{i,f} = 130.1\sigma$ $ \delta \bar{x}_3 _{i,f} = 118.4\sigma$
Case (2) subject to Eq.(13)	0.2, 1.7, 2.0 5.5, 46.0	Same as that in case (1)			
Case (3) subject to Eq.(16)	0.2, 1.8, 2.2 3.2, 45.0	37	$\delta \bar{k}_1 = \pm 2.96\sigma$ $\delta \bar{k}_2 = \pm 4.10\sigma$ $\delta \bar{k}_3 = \pm 2.24\sigma$ $\delta \bar{k}_4 = \pm 0.92\sigma$	$\delta J = +1146\sigma$	$ \delta \bar{x}_1 _{i,f} = 19.3\sigma$ $ \delta \bar{x}_2 _{i,f} = 128.9\sigma$ $ \delta \bar{x}_3 _{i,f} = 119.2\sigma$
Case (4) subject to Eq.(18)	0.2, 1.6, 1.9 5.4, 45.0	98	$\delta \bar{k}_1 = \pm 4.26\sigma$ $\delta \bar{k}_2 = \pm 4.24\sigma$ $\delta \bar{k}_3 = \pm 2.24\sigma$ $\delta \bar{k}_4 = \pm 0.90\sigma$	$\delta J = +1313\sigma$	$ \delta \bar{x}_1 _{i,f} = 23.2\sigma$ $ \delta \bar{x}_2 _{i,f} = 130.5\sigma$ $ \delta \bar{x}_3 _{i,f} = 118.8\sigma$
Case (5) subject to Eq.(19) ($i=3$, $s=4$)	0.2, 2.2, 3.4 7.9, 49.5	62	$\delta \bar{k}_1 = \pm 3.69\sigma$ $\delta \bar{k}_2 = \pm 4.51\sigma$ $\delta \bar{k}_3 = \pm 2.05\sigma$ $\delta \bar{k}_4 = \pm 0.824\sigma$	$\delta J = +1309\sigma$	$ \delta \bar{x}_1 _{i,f} = 22.4\sigma$ $ \delta \bar{x}_2 _{i,f} = 120.3\sigma$ $ \delta \bar{x}_3 _{i,f} = 108.9\sigma$
Case (6)	for example, 0.8, 2.2, 2.5 5.0, 48.5	11	$\delta \bar{k}_1 = \pm 4.59\sigma$ $\delta \bar{k}_2 = \pm 5.65\sigma$ $\delta \bar{k}_3 = \pm 2.61\sigma$ $\delta \bar{k}_4 = \pm 0.955\sigma$	$\delta J = +1556\sigma$	$ \delta \bar{x}_1 _{i,f} = 28.0\sigma$ $ \delta \bar{x}_2 _{i,f} = 146.5\sigma$ $ \delta \bar{x}_3 _{i,f} = 135.0\sigma$

minimum, and that the methods of case(3) or case(5) are desirable to determine the experimental conditions by which more reasonable values of parameters for process design can be estimated.

Furthermore, the results of case(6) show that experimental conditions selected arbitrarily may be inferior to the other cases.

3-6. CONCLUDING REMARKS

Methods to seek experimental conditions from which more reasonable values of parameters can be obtained were discussed^[3-7] . Particularly in this chapter, methods to select experimental conditions considering the influence of the estimated error of system parameters on the process design were proposed. A numerical example showed the effectiveness of these methods compared to methods minimizing the volume of the ellipsoid or of spherizing the ellipsoid.

NOMENCLATURE

J	; objective function defined by Eq.(3.23) [10^3cm^3]
k_i	; i-th dimensionless rate constant [-]
$\bar{k}_i$	; i-th real rate constant [1/min]
M_r	; covariance matrix of the error of observation
P_{ij}^{-1}	; (i,j) element of P^{-1}
q	; function shown in Eq.(3.15)
t	; time [min]
t_0	; initial time [min]
V	; tank reactor volume [10^3cm^3]
x_i	; dimensionless concentration [-]
$\bar{x}_i$	; real concentration of the i-th component [g/kg]
α	; vector of experimental conditions wich contain sampling time and α^o
α^o	; l -column vector of experimental conditions
b	; p-dimensional unit vector
H	; matrix given by Eq.(3.5)
P	; covariance matrix define by Eq.(3.5)
P_0^{-1}	; matrix defined by Eq.(3.12)
P_1^{-1}	; matrix defined by Eq.(3.17)
u	; design vector
α, β, γ	; constants given in Table 3.1
$\delta\theta$	; error of θ deviated from θ^*
θ	; weighting matrix defined by Eq.(3.11)
$\bar{\theta}$	; estiamted value of θ^*
θ^*	; true value of θ
λ_i	; eigenvalue of P^{-1}

λ_1^j ; eigenvalue of P_j^{-1} ($j=0,1$)

$\sigma^2 I$; covariance matrix of η_r in Eq. (3.22)

σ_b ; defined by Eq. (3.8)

τ ; dimensionless time [-]

Subscript

r ; value at sampling time t_r

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CHAPTER 4

DESIGN MARGIN TAKING INTO ACCOUNT

PARAMETER UNCERTAINTY - I

4-1. INTRODUCTORY REMARKS

Recently in the fields of chemical and sanitary engineering, the problem of how to determine the design variable, such as those at the scale of the plant, which maximizes or minimizes a certain objective function, that is, static optimal design problem, has been studied by using various mathematical optimization techniques.

It is not always sufficient to determine mathematical optimal values based only on mathematical models. The mathematical model used for optimization is constructed under appropriate assumptions, and the parameters which are included in the mathematical model have inevitable error in the estimation from the experiment or deviate more or less in an operational time. Thus, the determination of the optimal value of the design variable satisfying an optimal design problem, that is, the optimal design value, is not sufficient for a practical problem.

Usually a design margin or safety factor is added to or multiplied by the nominal design value in order to compensate for the undesira-

ble effects of the many uncertainties included in the design procedure and system operation, in spite of the fact that the nominal optimal design value is realized. Quantitative and rational evaluation of the design margin, however, has not been discussed sufficiently, especially for large complex process systems.

Recently, some methods for rationally determining the value of a design variable or for estimating the design margin accounting for parameter uncertainty have been studied. Most of those apply sensitivity analysis^{[4-1]~[4-10]}.

When separating these methods from calculation procedures, two divisions result. One called the "one-step Method" is used to determine the value of design variables by considering parameter uncertainty right from the beginning. The other which is called "the two-step Method" is used to determine the design margin to be added to the nominal optimum value which is designed based on the nominal value or mean value of uncertain parameters. The methods by Rudd^[4-1] and Rohrel^[4-2] use the one-step Method, and that by Takamatsu^[4-5] uses the two-step Method. Furthermore, when separating procedures from the information on parameter uncertainty, three classes result. One is when only the nominal value of parameter is known. The second is when the nominal value of the parameter and the range of parameter deviation are known. The third is when the probabilistic density function of parameter deviation is known. The information in this final class is the most plentiful of the three. In the same way as just described, the rational design methods accounting for parameter uncertainty are classified. A comparison of these methods is made in the latter of this chapter.

In this chapter at first, a new method of determining the design margin, taking the known probability density function of parameter deviation into account for plant design, is proposed. This method belongs to the two-step method class. It will be simple and easy to calculate design margin by the method proposed here because it introduces stochastic linear programming. Two numerical examples given show this method to be more reasonable than the one which utilizes only the ranges of parameter deviations.

Secondly, rational design methods for a process involving parameter uncertainty are compared by numerical calculation.

4-2. STATEMENT OF THE PROBLEM

Most large complex processes can be broken down into a number of subsystems. A typical subsystem is shown in Fig.4.1.

X_i is the input entering the i th subsystem from other subsystems, and M_i is a vector of decision variables in the i th subsystem manipulated to maximize or minimize a performance index. Z_i is the output from the i th subsystem going to other subsystems, while Y_i is the output from the i th subsystem which leaves the system and doesn't enter other subsystems. The values of Y_i are usually fixed as the conditions for the whole system design.

The subsystem is completely described, in the steady state, by giving its output as a function of its input.

$$Z_i = F_i(X_i, M_i, P_i) \quad (4.1)$$

$$Y_i = G_i(X_i, M_i, P_i) \quad i=1,2,\dots,N \quad (4.2)$$

where Z_i , Y_i , X_i and M_i are n_i , m_i , l_i and r_i dimensional vectors, and P_i is the vector of the nominal value of parameter which represents the characteristics of each subsystem. N is the total number of subsystems.

The total system is mathematically expressed by Equations (4.1) and (4.2), and the following condition of junction, which is a set of relations describing how the subsystems are interconnected,

$$X_i = \sum_{j=1}^N [C_{ij}] Z_j \quad (4.3)$$

where the matrixes $[C_{ij}]$ generally show which output of the j th subsystem is an input to the i th subsystem.

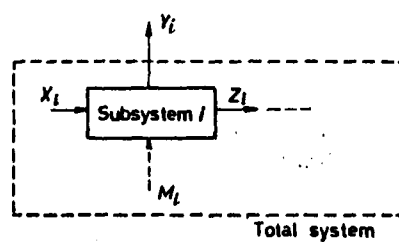


Fig. 4.1 Subsystem and total system.

The performance index of the whole system is assumed to be defined in separable form as follows,

$$F = \sum_{i=1}^N f_i(X_i, M_i) \quad (4.4)$$

The problem of the optimal design for this system is choosing M_i to minimize or maximize the performance index, F , subject to Eqs.(4.1), (4.2) and (4.3).

Introducing the adjoint variables, which are also called Lagrange multipliers, the following equations are obtained as a necessary condition,

$$\frac{\partial L}{\partial X_i} = \frac{\partial f_i}{\partial X_i} + \eta_i' \frac{\partial G_i}{\partial X_i} + \lambda_i' \frac{\partial F_i}{\partial X_i} - \pi_i' = 0 \quad (4.5)$$

$$\frac{\partial L}{\partial Z_i} = -\eta_i' + \sum_{j=1}^N \pi_j' [C_{ji}] = 0 \quad (4.6)$$

$$\frac{\partial L}{\partial M_i} = \frac{\partial f_i}{\partial M_i} + \eta_i' \frac{\partial G_i}{\partial M_i} + \lambda_i' \frac{\partial F_i}{\partial M_i} = 0 \quad (4.7)$$

$$\frac{\partial L}{\partial \eta_i} = F_i(X_i, M_i, P_i) - Z_i = 0 \quad (4.8)$$

$$\frac{\partial L}{\partial \lambda_i} = G_i(X_i, M_i, P_i) - Y_i = 0 \quad (4.9)$$

$$\frac{\partial L}{\partial \pi_i} = \sum_{j=1}^N [C_{ij}] Z_j - X_i = 0 \quad , \quad i=1,2,\dots,N \quad (4.10)$$

where L is the lagragian defined by

$$L = \sum_{i=1}^N \{ f_i + \eta_i' (F_i - Z_i) + \lambda_i' (G_i - Y_i) + \pi_i' (\sum_{j=1}^N [C_{ji}] Z_j - X_i) \} \quad (4.11)$$

and

$$\frac{\partial F_i}{\partial X_i} = \begin{bmatrix} \frac{\partial F_i^1}{\partial X_i^1} & \dots & \frac{\partial F_i^1}{\partial X_i^{n_i}} \\ \vdots & & \vdots \\ \frac{\partial F_i^{m_i}}{\partial X_i^1} & \dots & \frac{\partial F_i^{m_i}}{\partial X_i^{n_i}} \end{bmatrix}, \quad \frac{\partial F_i}{\partial M_i} = \begin{bmatrix} \frac{\partial F_i^1}{\partial M_i^1} & \dots & \frac{\partial F_i^1}{\partial M_i^{r_i}} \\ \vdots & & \vdots \\ \frac{\partial F_i^{m_i}}{\partial M_i^1} & \dots & \frac{\partial F_i^{m_i}}{\partial M_i^{r_i}} \end{bmatrix},$$

$$\frac{\partial f_i}{\partial X_i} = \begin{bmatrix} \frac{\partial f_i}{\partial X_i^1} & \dots & \frac{\partial f_i}{\partial X_i^{n_i}} \end{bmatrix}, \quad \frac{\partial f_i}{\partial M_i} = \begin{bmatrix} \frac{\partial f_i}{\partial M_i^1} & \dots & \frac{\partial f_i}{\partial M_i^{r_i}} \end{bmatrix},$$

$$\frac{\partial G_i}{\partial X_i} = \begin{bmatrix} \frac{\partial G_i^1}{\partial X_i^1}, \dots, \frac{\partial G_i^1}{\partial X_i^{n_i}} \\ \vdots \\ \frac{\partial G_i^{l_i}}{\partial X_i^1}, \dots, \frac{\partial G_i^{l_i}}{\partial X_i^{n_i}} \\ \frac{\partial G_i^1}{\partial X_i^1}, \dots, \frac{\partial G_i^{n_i}}{\partial X_i^{n_i}} \end{bmatrix}, \quad \frac{\partial G_i}{\partial M_i} = \begin{bmatrix} \frac{\partial G_i^1}{\partial M_i^1}, \dots, \frac{\partial G_i^1}{\partial M_i^{r_i}} \\ \vdots \\ \frac{\partial G_i^{l_i}}{\partial M_i^1}, \dots, \frac{\partial G_i^{l_i}}{\partial M_i^{r_i}} \\ \frac{\partial G_i^1}{\partial M_i^1}, \dots, \frac{\partial G_i^{r_i}}{\partial M_i^{r_i}} \end{bmatrix}$$

and ' denoted a vector transposed.

$$\eta_i^t = (\eta_i^1, \dots, \eta_i^{m_i}), \quad \lambda_i^t = (\lambda_i^1, \dots, \lambda_i^{l_i}),$$

$$\pi_i^t = (\pi_i^1, \dots, \pi_i^{n_i}),$$

are the adjoint variables for the equality constraints of Eqs. (4.1)~(4.3).

Application of Sensitivity Analysis to the Optimal Design of a Complex System :

The optimal design problem for a large complex system can be mathematically solved by applying some techniques, for example, the multilevel technique^{[4-11],[4-12]}. However in the application of mathematical techniques to deterministic design problems, it is generally assumed that the plant characteristics to be optimally designed for are exactly known, and plant parameters can be perfectly identified. However, often only the nominal values of the plant parameters and their range of variations are available, and the actual values of plant parameters differ from those used in mathematical computations for design. These differences are caused by the inaccuracies of predetermined parameter values or of the time-varying properties of the parameters. The difficulty in achieving an exact realization of optimum design variables should also be

considered in the problem of differences between calculation and practice. Therefore, from the engineering viewpoint, it may not be sufficient to obtain only the mathematical solution of the design problem formulated in Eqs.(4.1)~(4.4).

In actual design procedures, we usually take into account the design margin, or so-called "safety factor" of some design variables, to compensate for the bad influences of parameter variations. Moreover, it is desirable to estimate these design margins reasonably, so that the mathematical optimal design procedures may become more valuable from the practical viewpoint. For this purpose, we must know not only the effects of the parameter variations on the performance of the system but also what design margin must be estimated for each design variable to compensate for the bad effects.

Effect of Parameter Variations on Fixed Outputs [4-4],[4-5]:

Let us assume that the optimum design variables, M_i , which maximize the performance index of Eq.(4.4), have been mathematically determined. However, this optimal decision of M_i may force Y_i ($i=1, \dots, N$) to become a value which differs from the desirable value of Y_i , if the system parameters P_i is changed from the nominal values. Therefore, some design margin is usually taken into consideration in each design variable so that undersirable deviation of Y_i does not occur.

Let ΔM_i and ΔP_i , be the values of the design margin and parameter deviation from the nominal values in Eqs.(4.1) and (4.2), respectively. Under the condition of parameter deviation, the input and output variables, X_i , Z_i and Y_i deviate from the value at optimal conditions by the amount of ΔX_i , ΔZ_i and ΔY_i . The

relationship among these deviations, ΔX_i , ΔY_i , ΔZ_i , ΔM_i and ΔP_i can be easily ascertained without cumbersome direct computation by the help of the adjoint system which is introduced in the optimization procedure. The first-order variational equations are given by Eqs.(4.1)~(4.3) as follows:

$$\Delta Z_i = \frac{\partial F_i}{\partial X_i} \Delta X_i + \frac{\partial F_i}{\partial M_i} \Delta M_i + \frac{\partial F_i}{\partial P_i} \Delta P_i, \quad (4.12)$$

$$\Delta Y_i = \frac{\partial G_i}{\partial X_i} \Delta X_i + \frac{\partial G_i}{\partial M_i} \Delta M_i + \frac{\partial G_i}{\partial P_i} \Delta P_i, \quad (4.13)$$

$$\Delta X_i = \sum_{j=1}^N [C_{ij}] \Delta Z_j. \quad (4.14)$$

Summing up over i both sides of Eqs.(4.12)~(4.14) multiplied by the adjoint variables α_i , β_i and γ_i which are m_i , l_i and n_i dimensional, respectively, the following equation is obtained,

$$\begin{aligned} \sum_{i=1}^N \beta'_i \Delta Y_i &= \sum_{i=1}^N [(\alpha'_i \frac{\partial F_i}{\partial X_i} + \beta'_i \frac{\partial G_i}{\partial X_i} - \gamma'_i) \Delta X_i + (-\alpha'_i + \sum_{j=1}^N \gamma'_j [C_{ji}]) \Delta Z_i \\ &\quad + (\beta'_i \frac{\partial G_i}{\partial M_i} + \alpha'_i \frac{\partial F_i}{\partial M_i}) \Delta M_i] \\ &\quad + \sum_{i=1}^N (\alpha'_i \frac{\partial F_i}{\partial P_i} + \beta'_i \frac{\partial G_i}{\partial P_i}) \Delta P_i. \end{aligned} \quad (4.15)$$

By using the solution of the adjoint system defined by

$$\alpha'_i \frac{\partial F_i}{\partial X_i} + \beta'_i \frac{\partial G_i}{\partial X_i} - \gamma'_i = 0 \quad (4.16)$$

$$-\alpha'_i + \sum_{j=1}^N [C_{ij}]' \gamma_j = 0 \quad (4.17)$$

with the boundary conditions of

$$\begin{aligned} \beta_n^m &= 1, \quad \beta_n^j = 0 & j &\neq m \\ & & i &\neq n \\ \beta_i^j &= 0 & j &= 1, 2, \dots, l_i \end{aligned} \quad (4.18)$$

the following equation is obtained from Eq.(4.15):

$$\Delta Y_n^m = \sum_{i=1}^N \left\{ [(\beta_i)' \frac{\partial G_i}{\partial M_i} + (\alpha_i)' \frac{\partial F_i}{\partial M_i}] \Delta M_i + [(\alpha_i)' \frac{\partial F_i}{\partial P_i} + (\beta_i)' \frac{\partial G_i}{\partial P_i}] \Delta P_i \right\} \quad (4.19)$$

where $(\beta_i)_{nm}$ and $(\alpha_i)_{nm}$ are the solution of the adjoint systems^[4-19].

This equation denotes the deviation of the m th component of the system output in the n th subsystem from the desirable output value.

As stated above, it is necessary for actual design of a plant to determine rationally the value of the design variable or to estimated the design margin accounting for parameter uncertainty.

Here a method of estimating design margin taking into account parameter uncertainty when the probability density function of parameters P_i is known is proposed at first. The method is an extension of a two-step method by T. Takamatsu et al^[4-5]. Knowing the probability density function of parameters, P_i is the same as knowing the probability density function of the deviation of parameters, ΔP_i from nominal value $\bar{P}_i$. It is the purpose of the next section of give the mothod of evaluating the rational design margin based on the known probability density function of ΔP_i .

4-3. DESIGN MARGIN BY THE TWO-STEP METHOD

The design margin by the two-step method is determined as follows: First, the nominal optimum design value of design variables, $\bar{M}_i$, are obtained based on nominal values of the parameters, $\bar{P}_i$ by using multilevel or other techniques. Next, the rational design margin ΔM_i to be added to the nominal optimum design value $\bar{M}_i$ is determined based on the information of the known probability density function of ΔP_i . The final value of the design variable variable becomes $\bar{M}_i + \Delta M_i$.

The method of evaluating the design is given as follows: When parameters P_i deviate by ΔP_i , an allowable region is usually given to the perturbation of the system output, ΔY_n , to be fixed due to undesirable perturbations of the parameters. Then, design margin ΔM_i is determined so as to minimize some objective function, h , constructed by ΔM_i under the condition of ΔY_n being in the allowable range. h represents the cost of evaluating the design margin. For example, if M_i is the amount of the catalyst of the chemical reactor, h may be the cost of the excess catalyst or the increase of reactor volume. If M_i is the heat transfer area of the heat exchange system, h is the increase of the construction cost or operating cost needed to add the design margin ΔM_i to $\bar{M}_i$. On the other hand, in a chemical reactor, the upper limit $C_{U,i}$ and lower limit $C_{L,i}$ of the allowable ranges of the deviation of system output to be fixed correspond to the allowable ranges of output concentration of the desirable

product.

The relations between ΔY_n , ΔP_i and ΔM_i are given by Eq. (4.19). Then the design margin ΔM_i is determined by Eq. (4.20) based on Eq. (4.16)~(4.19) and Eq. (4.21).

$$\text{Min}_{\{\Delta M_i\}} \{h = h(\Delta M_1, \dots, \Delta M_N)\} \quad (4.20)$$

$$C_{L,n} \leq \Delta Y_n \leq C_{U,n} \quad , \quad n=1,2,\dots,N \quad (4.21)$$

$$\Delta M_i \geq 0$$

where h , $C_{L,i}$ and $C_{U,i}$ are the known functions and known constant vectors, respectively. When the upper and lower limits of ΔP_i are given, ΔP_i is subjected to next equation,

$$A_{L,i} \leq \Delta P_i \leq A_{U,i} \quad i=1,2,\dots,N \quad (4.22)$$

where $A_{U,i}$ and $A_{L,i}$ are the given constant vectors.

If h is a linear function of ΔM_i , the problem of design margin by Eqs. (4.16)~(4.21) is reduced to a L.P. (linear programming) problem where ΔP_i in Eq. (4.19) is taken as $A_{U,i}$ or $A_{L,i}$.

ΔP_i^j which is the j -th component of ΔP_i should be chosen as $A_{U,i}^j$ or $A_{L,i}^j$ so that the deviation of ΔP_i^j causes an undesirable effect on ΔZ_i . For example, let us consider the case in which the following equations can be written for Eq. (4.19),

$$\Delta Y_n^1 = b_1 \Delta M_1^1 + d_1 \Delta P_1^1 + e_1 \Delta P_1^2 + \dots \quad (4.19)'$$

$$\Delta Y_n^2 = b_2 \Delta M_1^1 + d_2 \Delta P_1^1 + e_2 \Delta P_1^2 + \dots$$

The allowable ranges of ΔY_n^1 and ΔY_n^2 are given by,

$$\begin{aligned}\Delta C_{L,n}^1 &\leq \Delta Y_n^1 \leq \Delta C_{U,n}^1 \\ \Delta C_{L,n}^2 &\leq \Delta Y_n^2 \leq \Delta C_{U,n}^2\end{aligned}\tag{4.21}'$$

$\Delta C_{L,n}^i$ usually is a negative value and the constraint of ΔY_n sometimes needs either the upper or lower bound only. It cannot

generally be known whether ΔP_i^j is negative or positive value.

In some cases, it may be clear that P_i^j changes dynamically in one direction from the nominal value of $\bar{P}_i^j$. Assuming that d_1 and e_1 are positive values and that ΔY_n^1 must not be above the positive value of $\Delta C_{U,n}^1$, ΔP_1^1 and ΔP_1^2 must take $A_{L,1}^1$ and $A_{L,1}^2$ respectively.

Assuming that d_2 and e_2 are negative and positive values, respectively and that ΔY_n^2 must be greater than the negative value of $\Delta C_{L,n}^2$, ΔP_1^1 and ΔP_1^2 must be taken as $A_{L,1}^1$ and $A_{U,1}^2$, respectively. Practically it does not happen that ΔP_1^2 is simultaneously $A_{L,1}^1$ and ΔY_n^1 and $A_{U,1}^2$ for ΔY_n^2 , but the above treatment gives a result on the safe side.

This is the two-step method given by T. Takamatsu et al^[4-5], when the range of parameter deviation is given.

Now we consider the case in which the probability density function of ΔP_i^j is known. In this case, the methods of slack solution and fat solution which are the methods of stochastic programming^{[4-14]~[4-18]} considered for parameter uncertainty are applied to the design margin problem. The method of fat solution, however, can be reduced to the two-step method when the upper and lower limits of parameter deviation are given.

Slack solution

According to the idea of slack solution^[4-17], the inequality constraint of ΔY_n given by Eq. (4.21) is reduced to an equality constraint by introducing non-negative values $y_{i1}, y_{i2}, y_{i3}, y_{i4}$ termed "slack variables" as follows:

$$\begin{aligned} \Delta Y_i + y_{i1} - y_{i2} &= C_{L,i} \\ \Delta Y_i + y_{i3} - y_{i4} &= C_{U,i} \\ y_{ij} &\geq 0 \\ j &= 1, 2, \dots, N \\ \Delta M_i &\geq 0 \\ i &= 1, 2, \dots, 4 \end{aligned} \quad (4.23)$$

As values of y_{i1}, y_{i4} are positive only when inequality constraint Eq. (4.21) is not satisfied, the new objective function Φ ,

$$\Phi = h(\Delta M_1, \dots, \Delta M_N) + \sum_{i=1}^N (\mu_{i1}^T y_{i1} + \mu_{i4}^T y_{i4}) \quad (4.24)$$

is introduced. The design margin ΔM_i is determined so as to minimize the expected value of Φ given by Eq. (4.24), that is, ΔM_i is determined by solving the next equation,

$$\text{Min}_{\substack{\{\Delta M_i\} \\ \{y_{ij}\}}} \left\{ E_{\substack{P^i}} [\Phi = h(M_1, \dots, M_N) + \sum_{i=1}^N (\mu_{i1}^T y_{i1} + \mu_{i4}^T y_{i4})] \right\} \quad (4.25)$$

where, $E_{\substack{P^i}} []$ represents the expected value with respect to probability density function P^i , and μ_{ij} ($i=1, 2, \dots, N, j=1, 4$) are constant vectors. The probability density function of P^i is given as

$$P^P i = P^P i (\Delta P_i) \quad (4.26)$$

$$i = 1, 2, \dots, N$$

The second term of Eq. (4.24) or Eq. (4.25) represent a penalty cost which evaluates the quantitative degree of dissatisfaction of the inequality constraint, Eq. (4.21). μ_{i1}, μ_{i2} are coefficients of penalty cost. For example, if h in Eq. (4.25) represents production cost, μ_{i1}, μ_{i4} are unit costs caused by the unit amount of increasing or decreasing the output vector Y_i . That is, μ_{i1} and μ_{i2} are practical values. It is then practical to determine the design margin by using Eq. (4.25).

If function h is linear with respect to ΔM_i , Eq. (4.25) can be rewritten as follows,

$$\text{Min}_{\{\Delta M_i\}} \{ \phi = h(\Delta M_1, \dots, \Delta M_N) + E[\text{Min}_{\{P^P i\}} (\sum_{i=1}^N (\mu_{i1}^T y_{i1} + \mu_{i4}^T y_{i4}))] \} \quad (4.27)$$

The design margin ΔM_i can be determined by solving Eq. (4.25) or Eq. (4.27) under the conditions of Eq. (4.16)~(4.19) and (4.23) when probability density function of ΔP_i , which is deviation of parameters from nominal value $\bar{P}_i$ is known.

Fat solution

According to the concept of fat solution^[4-18], the design margin ΔM_i is determined so as to minimize the objective function h when the probability of inequality constraint being satisfied is greater

than a certain given value. That is, ΔM_i can be determined by solving Eq.(4.28) subject to Eqs.(4.16)-(4.19) and (4.29).

$$\begin{aligned} \text{Min}_{\{\Delta M_i\}} h(\Delta M_1, \dots, \Delta M_N) \quad (4.28) \\ i=1, 2, \dots, N \end{aligned}$$

$$\text{Pr}_{\{P_i^j\}} \{C_{L,i}^j \leq \Delta Y_i^j \leq C_{U,i}^j\} \geq \beta_i^j \quad j=1, 2, \dots, l_i \quad (4.29)$$

where the superscript j represents the j -th component and β_i^j is a given constant which satisfies the condition $0 \leq \beta_i^j \leq 1$. The value of β_i^j depends on the degree of importance of the inequality constraint, Eq.(4.21). Pr in Eq.(4.29) represents probability. ΔY_i in Eq.(4.29) is the linear function of ΔP_i , as shown in Eq.(4.19). If ΔP_i ($i=1, \dots, N$) is statistically independent, Eq.(4.29) becomes a simple inequality equation which is reduced by substituting the upper or lower value of the confidence interval of confidence level β_i into ΔP_i , in Eq.(4.29). For example, if the values of the confidence limits are e_{pi} , and each component of e_{pi} and coefficient vector multiplied to ΔP_i in Eq.(4.19) are positive, Eq.(4.29) can be rewritten as follows

$$\begin{aligned} \sum_{i=1}^N (\alpha_i^T \frac{\partial F_i}{\partial M_i} + \beta_i^T \frac{\partial G_i}{\partial M_i}) \Delta M_i - \sum_{i=1}^N (\alpha_i^T \frac{\partial F_i}{\partial P_i} + \beta_i^T \frac{\partial G_i}{\partial P_i}) e_{pi} \geq C_{L,n}^m \\ \sum_{i=1}^N (\alpha_i^T \frac{\partial F_i}{\partial M_i} + \beta_i^T \frac{\partial G_i}{\partial M_i}) \Delta M_i + \sum_{i=1}^N (\alpha_i^T \frac{\partial F_i}{\partial P_i} + \beta_i^T \frac{\partial G_i}{\partial P_i}) e_{pi} \leq C_{U,n}^m \end{aligned} \quad (4.30)$$

where α_i , β_i satisfy Eqs.(4.16)~(4.18).

Then, ΔM_i can be determined by solving Eq.(4.28) when the conditions of Eqs.(4.16)~(4.19) and (4.29) are reduced to determine the design margin ΔM_i and when the upper or lower limit of parameter deviation ΔP_i is given.

As stated above, the design margin ΔM_i can be determined rationally when probability density functions of ΔP_i is known. That is, the solution is obtained by solving Eq.(4.25) or Eq.(4.28) under the condition of Eqs.(4.16)-(4.19) and Eq.(4.23). The method of determining the design margin ΔM_i based on Eq.(4.25) or Eq.(4.28) is the one proposed here. Because based on the method, the relations between the deviation of the system output vector, the deviation of parameter, ΔP_i and design margin ΔM_i are approximated by linear relations, and because these relations can easily be reduced by using adjoint variables, calculation by the method is comparatively easy.

On the other hand, the probability density function of parameter deviation may be estimated for the most part by incorporation of experimental data, especially when the estimation error of the parameter becomes a normal distribution. The method proposed here is more practical in spite of the fact that the probability density function must be known beforehand. Also by this method the design margin to be estimated is less than by other two step methods only when the range of parameter deviation is known.

When the probability density function is not symmetrical, it is doubtful that the method proposed here will be useful. This problem will be discussed further.

4-4. EXAMPLE-1

An application to a Wet-air oxidation process^{[4-19],[4-20]}, is one of the methods of treating excess sludge from a waste-water treatment process. Oxidation^[4-16] proceeds in Wet-air oxidation of sewage sludge. The reactor is a completely mixed tank type held at a steady state.

Where the reaction model is given in Fig.4.2. A represents sludge. B and C represents the intermediate product and P is the final product. Reaction order of each path is assumed to be of the first order. Denoting the flow rate, tank volume, inlet concentrations of each component and outlet concentrations by F , V , C_{A0} , C_{B0} , C_{C0} , C_{P0} , C_A , C_B , C_C , and C_P , respectively, the process equation is

$$F(C_{i0} - C_i) - r_i \cdot \rho V = 0 \quad , \quad i = A, B, C, P \quad (4.31)$$

where, ρ is the density of outlet flow and is taken as 1.0, r_i is the chemical reaction rate given by

$$\begin{bmatrix} r_A \\ r_B \\ r_C \\ r_P \end{bmatrix} = \begin{bmatrix} -(k_1 + k_2), & 0 & , & 0 & , & 0 \\ k_1 & , & -(k_3 + k_5), & k_4 & , & 0 \\ k_2 & , & k_3 & , & -(k_4 + k_6), & 0 \\ 0 & , & k_5 & , & k_6 & , & 0 \end{bmatrix} \begin{bmatrix} C_A \\ C_B \\ C_C \\ C_P \end{bmatrix} \quad (4.32)$$

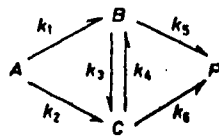


Fig. 4.2 Reaction model of wet-air oxidation of sludge.

Table 4.1 Nominal optimal design for Example-1.

Estimated parameter value [1/min]	Assumed value	Nomin. Opt. design
$k_1=0.230, k_2=0.121, k_3=0.003$	$F=100[\text{kg/min}], \alpha=0.01[1/10^3\text{cm}^3]$	$V_{\text{opt}}=10[\text{m}^3]$
$k_4=0.00007, k_5=0.014, k_6=0.0004$	$\beta=50[\text{kg/g}], C_{A0}=15[\text{g/kg}]$	$\bar{C}_P=7.7[\text{g/kg}]$
	$C_{B0}=5[\text{g/kg}], C_{C0}=C_{P0}=0.0$	$J=715[-]$

where k_i is the chemical reaction rate constant. As P is the final form of sludge treated by Wet-air oxidation (H_2O , CO_2 , etc.), it is desirable to produce P as much as possible from the viewpoint of sludge treatment. On the other hand, if we want to produce more P , greater tank volume of the reactor, V is required, and construction and operating costs become greater. Then, we will choose a V which minimizes the objective function J given by Eq.(4.33) subjected to Eqs.(4.31) and (4.32).

$$J = \alpha V + \beta(C_{A0} + C_{B0} - C_P) \quad (4.33)$$

where α and β are the coefficients used for calculating operating and construction costs. Cost is represented by a dimensionless number.

The reaction rate constants in Eq.(4.32) which are parameters estimated from experimental data involve inevitable error. Only k_1 and k_2 are assumed to involve error. The problem considered here is to evaluate the design margin ΔV which must be added to the nominal optimum design by considering the known probability density function of the uncertain parameter deviation Δk_1 , Δk_2 , in order to decrease the worse effects of such parameter deviation on the output concentration of the product, C_P .

Now, we assume that 144 tons/day of sludge of which about 97.9% contains water is treated. The nominal parameter value $\bar{k}_1 \sim \bar{k}_6$, and other numerical values used here are listed in Table 4.1^[4-20]. The nominal optimum design value based on the estimated parameter value $\bar{k}_1 \sim \bar{k}_6$ is calculated as follows, $\bar{V}_{opt} = 10m^3$, $\bar{J} = 715$, $\bar{C}_P = 7.7[g/kg]$. We impose such a condition so that the deviation of the

concentration of the product P will not be less than 5.0% of the nominal optimum value $\bar{C}_p$ even if the parameter deviation $\Delta k_1, \Delta k_2$ exist. The condition is, $\Delta C_p / \bar{C}_p \geq -0.05$. The relation between ΔC_p , Δk_1 and Δk_2 is introduced in this condition. Then, the next condition

$$7.63\Delta k_1 - 12.0\Delta k_2 + 3.22 \times 10^{-4} \Delta V \geq -0.385 \quad (4.34)$$

is deduced.

Now, let's assume that the design margin ΔV is taken as h in Eq. (4.20),

$$\text{Min } \{h=\Delta V\} \quad (4.35)$$

and determine ΔV by using Eq. (4.27) and the probability density function $\Delta k_i, P^{ki}(\Delta k_i)$. It is known that Δk_1 and Δk_2 have normal distribution with zero mean and variance σ_1, σ_2 ($\sigma_1 = 0.0408, \sigma_2 = 0.00204^{[4-20]}$). For the comparison, however, three cases of the probability density function of $\Delta k_1, \Delta k_2$ as follows are considered as an approximate form of that normal distribution: Case i) uniform distribution; Case ii) triangular distribution with the same upper and lower limit as case i) for comparison with the solution of the case i); and case iii) a triangular distribution which is an approximation of the normal distribution. The design margin ΔV based on case i)-case iii), respectively, is calculated as follows, and the calculation in case i) is explained, more fully.

Case i):—Uniform Distribution—

Δk_1 and Δk_2 are uniformly distributed in the range of 95% confidence interval. That is, the probability density function of

Δk_i , $P^{ki}(\Delta k_i)$ is given by

$$P^{ki}(\Delta k_i) = \begin{cases} \frac{1}{3.92\sigma_i} & , \text{for } |\Delta k_i| \leq 1.96\sigma_i \\ 0 & , \text{for } |\Delta k_i| > 1.96\sigma_i \end{cases} \quad (4.36)$$

where $\sigma_1 = 0.0408$, $\sigma_2 = 0.00204$. According to Eq.(4.27), design margin ΔV is calculated as follows, and by introducing slack variables y_1, y_2 , Eq.(4.34) becomes,

$$\begin{aligned} 7.63\Delta k_1 - 12.0\Delta k_2 + 3.22 \times 10^{-4} \Delta V + y_1 - y_2 &= -0.385 \\ y_1 \geq 0, \quad y_2 \geq 0 \end{aligned} \quad (4.37)$$

Modified new objective function Φ is defined as

$$\Phi = \Delta V + \mu y_1 \quad (4.38)$$

where μ is taken as 10^5 . First the minimum value of μy_1 is

$$\text{Min}(\mu y_1) = \begin{cases} 0 & , \text{for } \Delta V \geq \frac{-0.385 - 7.63\Delta k_1 + 12.08\Delta k_2}{3.22 \times 10^{-4}} \\ \mu(-0.385 - 7.63\Delta k_1 + 12.0\Delta k_2 - 3.22 \times 10^{-4} \Delta V) & \text{for } \Delta V < \frac{-0.385 - 7.63\Delta k_1 + 12.08\Delta k_2}{3.22 \times 10^{-4}} \end{cases} \quad (4.39)$$

Next, the expected value of $[\text{Min}(\mu y_1)]$ is given as

$$E_{\{P^{ki}\}} [\text{Min}(\mu y_1)] = \begin{cases} 0 & , \text{for } \Delta V \geq 850, \\ 781.25\mu[-60.87 \times 10^{-15} \Delta V^3 + 1.56 \times 10^{-10} \Delta V^2 - 1.314 \times 10^{-7} \Delta V + 3.7 \times 10^{-5}] & , \text{for } 550 \leq \Delta V < 850, \\ 781.25\mu[0.548 \times 10^{-10} \Delta V^2 - 0.76 \times 10^{-7} \Delta V + 0.273 \times 10^{-5}] & , \text{for } 0 \leq \Delta V < 550. \end{cases} \quad (4.40)$$

The result, $\text{Min}_{\Delta V} [\Phi = \Delta V + E_{\{P^{ki}\}} [\text{Min}(\mu y_1)]] = 697[1]$ at $\Delta V = 625[1]$.

Then the design margin ΔV is given as 625[7].

Case ii):—Triangular Distribution-1—

We consider the case in which the probability density function of $\Delta k_i (i=1,2)$ is given as a triangular distribution with the same upper and lower limit as in case i) for comparing the effect of the difference of probability density function of the design margin to be evaluated. The probability density function is given as follows,

$$P^{k_i}(\Delta k_i) = \begin{cases} -\frac{1}{(1.96\sigma_i)^2} \cdot |\Delta k_i| + \frac{1}{1.96\sigma_i}, & \text{for } |\Delta k_i| \leq 1.96\sigma_i \\ 0 & \text{for } |\Delta k_i| > 1.96\sigma_i \end{cases}$$

$$i=1,2, \quad \sigma_1=0.0408, \sigma_2=0.00204. \quad (4.41)$$

In this case, the design margin to be added is calculated as $\Delta V = 322[7]$ in the same way as case i).

Case iii):—Triangular Distribution-2—

A triangular distribution which is the least square approximation of normal distribution is given as,

$$P^{k_i}(\Delta k_i) = \begin{cases} -\frac{1}{(2.31\sigma_i)^2} \cdot |\Delta k_i| + \frac{1}{2.31\sigma_i}, & \text{for } |\Delta k_i| \leq 2.31\sigma_i \\ 0 & \text{for } |\Delta k_i| > 2.31\sigma_i \end{cases}$$

$$i=1,2, \quad \sigma_1=0.0408, \sigma_2=0.00204. \quad (4.42)$$

The design margin is calculated as $\Delta V = 579[7]$ in the same way as in case i).

These results are listed in Table 4.2. The design margin calculated by Fat solution is also listed in Table 4.2 where Δk_1 and Δk_2 are assumed to have normal distribution with zero mean and

Table 4.2 Design margin for Example-1.

		Prob. dens. func.	μ	Design margin
Design margin for $\delta C_p/\bar{C}_p \geq -0.05$	Adjoint Method, Eq. (18)	case(i) Eq.(27) variance :	10^5	$\delta V=0.625 \text{ [m}^3\text{]}$
		$\delta k_1; 21.3 \times 10^{-4}$	∞	$\delta V=0.850 \text{ [m}^3\text{]}$
		$\delta k_2; 5.3 \times 10^{-6}$		
		case(ii) Eq. (32) variance :	10^5	$\delta V=0.322 \text{ [m}^3\text{]}$
		$\delta k_1; 10.7 \times 10^{-4}$	∞	$\delta V=0.850 \text{ [m}^3\text{]}$
		$\delta k_2; 2.7 \times 10^{-6}$		
	Fat. Sol. Eq. (19) (20)	case(iii) Eq.(33) variance :	10^5	$\delta V=0.579 \text{ [m}^3\text{]}$
		$\delta k_1; 14.8 \times 10^{-4}$	∞	$\delta V=1.210 \text{ [m}^3\text{]}$
		$\delta k_2; 3.7 \times 10^{-6}$		
		normal dist. $\sigma_{k1}=0.0408$ $\sigma_{k2}=0.00204$		

variance $\sigma_i^2 (i=1,2)$. The standard deviation σ_1 and σ_2 are taken as $\sigma_1 = 0.04-8$, $\sigma_2 = 0.00204$ and β in Eq.(4.29) is assumed to be 0.95.

The following becomes clear from Table 4.2;

The difference in the probability density function of Δk_i causes the difference of the design margin to be added even if the mean value of Δk_i and the coefficient of penalty cost, μ , are the same. In this case, the variance of each probability density function is naturally different. For example, let's compare case i) and case ii) where in both cases the mean value of Δk_i is zero, and the ranges of the deviation Δk_i are within the same interval, $1.96 \sigma_i (i=1,2)$, but the variance Δk_i is different in both cases. It becomes clear from Table 4.2 that the design margin in the triangular distribution (case ii)) is about half as large as that in the uniform distribution (case i)). It may be reasonable from the fact that the variance of the uniform distribution is larger than that of the triangular distribution. Then, the information about the probability density function of the parameter deviation is more important than that of the range of the parameter deviation which decreases the design margin to some extent.

By comparing case ii) and case iii), it is clear that the design margin becomes greater as the range of the parameter deviation Δk_i for which probability density function is triangular becomes greater, that is, the variance of Δk_i becomes greater. When $\mu \rightarrow \infty$, y_1 must be equal to zero, that is, the inequality constraint, Eq.(4.34), must be satisfied for all $\Delta k_i (i=1,2)$. In this case, the design margin is the same when the range of parameter deviation is used, but the distribution of Δk_i is not considered.

Then, the design margin to be added is the same in both case i) and case ii) for $\mu=\infty$. The solution becomes $\Delta V = 850[7]$. The range of parameter deviation in case i) and ii) is taken to be equal to the 95% confidence interval, When Δk_i has a normal distribution, the design margin calculated by the method of the Fat solution using Eqs.(4.29),(4.29) where the probability of satisfying an equality constraining Eq.(4.34) is taken as 95% is coincidence with that of case i) and ii) for $\mu=\infty$. The design margin by the method of fat solution results in a situation when only the range of parameter deviation is known, and the range of case i) or ii) is the same as that in the case of the method of Fat solution.

4-5. EXAMPLE-2

We consider the static optimum design of the counter current heat exchange system^[4-21] shown in Fig.4.3. R_{ij} , S_{ij} , G_{ij} , and T_{ij} are input and output temperatures of cold and hot streams at the ij -th sub-unit, respectively. W_{ij} and w_{ij} represent flow rates, and C_p , C'_p represents specific heat, where the nomenclature for hot stream is W_{ij} , C_p . Now we assume that $W_{ij} C_p = w_{ij} C'_p \triangleq WC_p$ ($i=1,2$, $j=1,2$). This assumption is that both hot and cold stream have the same heat flow rate ($W \cdot C_p$) and is very important for reducing systems equations. Now denoting the heat transfer area as A_{ij} , and the overall heat transfer coefficient as U_{ij} , the system equations are given as

$$S_{ij} = \frac{R_{ij} + U_{ij} A_{ij} G_{ij} / WC_p}{1 + U_{ij} A_{ij} / WC_p} \quad (4.43)$$

$$T_{ij} = R_{ij} + G_{ij} - S_{ij} \quad i=1,2, \quad j=1,2.$$

The inlet temperature of the hot stream is given, and the outlet temperature are not fixed. When the flow rate and the inlet and outlet temperatures of the cold streams are given as fixed values, find the A_{ij} , surface area of the heat exchanger, that minimizes the following objective function,

$$J = \sum_{i,j=1}^2 A_{ij} \quad (4.44)$$

J means the total surface area of the heat exchangers and corresponds to investment cost. The nominal values of the parameters

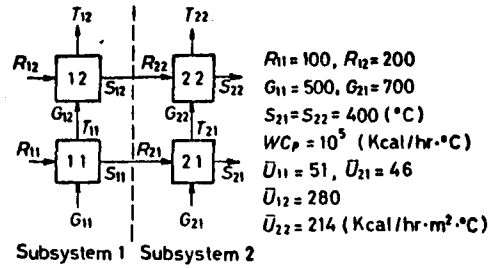


Fig. 4.3 Heat exchanger system.

Table 4.3 Design margin for Example-2.

Nominal optimal design		$A_{11}=994, A_{12}=110, A_{21}=1232, A_{22}=575 \text{ [m}^2\text{]}$
Design margin for Eq. (39)	case(i) $\mu_{21} = \left(\frac{\mu}{\mu}\right)$	$0 \leq \mu \leq 13.4 \quad ; \quad \partial A_{ij} = 0$
		$13.4 < \mu \leq 15.1 \quad ; \quad \partial A_{11} = \partial A_{12} = \partial A_{22} = 0, \partial A_{21} = 319 - \frac{4279}{\mu}$
		$15.1 < \mu \quad ; \quad \partial A_{11} = 0, \partial A_{12} + \partial A_{22} = 139 - \frac{2102}{\mu}, \partial A_{21} = 319 - \frac{4279}{\mu}$
	case(ii) $\mu_{21} = \left(\frac{\mu}{\mu}\right)$	$\mu = 0 \quad ; \quad \partial A_{ij} = 0$
		$\mu = 10^3 \quad ; \quad \partial A_{11} = \partial A_{12} = \partial A_{22} = 0, \partial A_{21} = 228.5$
		$\mu = \infty \quad ; \quad \partial A_{11} = 0, \partial A_{12} + \partial A_{22} = 170, \partial A_{21} = 377$

U_{ij} which is the total heat transfer coefficient is used, and the other numerical values necessary to solve the nominal optimum design described above are listed in Fig.4.3. The nominal optimum design to minimize J in Eq.(4.44) subjected to Eq.(4.43) is calculated as shown in the first row of Table 4.3.

Next, we evaluate the design margin which may be necessary to compensate for the undesirable effects of parameter deviation on the output temperature of cold stream when parameters U_{ij} have estimation error or deviate to some extent during the operating period.

The relations between the parameter deviation, ΔU_{ij} , from nominal value ΔU_{ij} , the design margin of the surface area of the heat exchanger, ΔA_{ij} , and the output temperature deviation of the cold stream, ΔS_{21} , S_{22} , are given as follows from Eqs.(4.16)-(4.19).

$$\begin{bmatrix} \Delta S_{21} \\ \Delta S_{22} \end{bmatrix} = \begin{bmatrix} -0.0575, & 0.0882, & 0 \\ 0.0084, & -0.0486, & 0.125 \end{bmatrix} \begin{bmatrix} \Delta A_{11} \\ \Delta A_{21} \\ \Delta A_{12} + \Delta A_{22} \end{bmatrix} + \begin{bmatrix} 57.12, & 108.56, & 0, & 0 \\ 8.313, & -59.8, & 13.72, & 72.12 \end{bmatrix} \begin{bmatrix} \Delta U_{11} \\ \Delta U_{21} \\ \Delta U_{12} \\ \Delta U_{22} \end{bmatrix} \quad (4.45)$$

where ΔU_{ij} is made a dimensionless value as follows,

$$\Delta U_{ij} = \frac{\Delta U_{ij}}{\bar{U}_{ij}}, \quad i=1,2, \quad j=1,2. \quad (4.46)$$

We now consider the following problem:

When the probability density function of ΔU_{ij} is known, the design margin ΔA_{ij} is determined so as to make the decrease of the output temperature of the cold stream less than 5°C and to minimize the sum of the design margin. That is, we determine ΔA_{ij} which minimizes h in Eq.(4.47) subjected to Eq.(4.48).

$$h = \sum_{i,j=1}^2 \Delta A_{ij} \quad (4.47)$$

$$\Delta S_{2i} \geq -5, \quad i=1,2. \quad (4.48)$$

This problem is solved by introducing slack variable Y_{2j} in the same way as Example-1 and by using Eq.(4.27). We consider the following two types as the probability density function of ΔU_{ij} ,

Case i) Uniform Distribution:

The value of the total heat transfer coefficient U_{ij} becomes smaller as long as the operation time increases because, for example, the scale is given. If U_{ij} decreases linearly with respect to operation time, ΔU_{ij} may be considered to be uniformly distributed from 0 to some negative value.

The manner of decrease of ΔU_{ij} and ΔU_{mn} is the same so we can consider that $\Delta U_{ij} = \Delta U$. In numerical calculation, ΔU is distributed uniformly from 0 to -0.2. Naturally, the mean value of ΔU is not zero.

Case ii) Triangular Distribution

The deviation of parameter U_{ij} from the nominal value, ΔU_{ij} , generally has a normal distribution^[4-22] when the parameters are estimated from experimental data. In actual calculation, the normal distribution is approximated by triangular distribution $P^{U_{ij}}(\Delta U_{ij})$

shown in Eq.(4.42), and the triangular distribution is used where $\sigma_{ij}=0.1$ is used.

The results calculated by Eq.(4.27) are listed in Table 4.3.

We now compare case (i) and (ii) for $\mu=10^3$. In case (i), the solution is; $\Delta A_{11}=0$, $\Delta A_{12}+\Delta A_{22}=137$, $\Delta A_{21}=315$, on the other hand, in case (ii), the solution is; $\Delta A_{11}=\Delta A_{12}=\Delta A_{22}=0$, $\Delta A_{21}=228.5$. Then the sum of the design margins for a triangular distribution (case (ii)) may be clearly less than that for a uniform distribution (case (i)). This result may come from the fact that ΔU_{ij} in case (i) is distributed from -0.2 to 0 and ΔU_{ij} in case (ii) is distributed from -0.231 to 0.231; that is, the mean value of ΔU_{ij} in case (ii) is larger than that in case (i) (mean value of ΔU_{ij} in case (i) is -0.1 and that in case (ii) is 0).

When we test case (i), the sub-unit to which the design margin must be added is different as μ becomes greater. For example, the design margin is zero for every sub-unit for $\mu \leq 13.4$. The sub-unit to which the design margin must be added is only the 21-st unit for $13.4 < \mu \leq 15.1$. The sub-units to which design margin must be added are the 21-st unit and 12-th or 22-nd unit when μ is greater than 15.1. In this case, design margins are not uniquely determined, but the sum of ΔA_{12} , and ΔA_{22} are given because linear stochastic programming is not uniquely determined. As μ becomes greater, design margins come close to the solution; $\Delta A_{11}+\Delta A_{22}=139$, $\Delta A_{21}=319$ which is the solution when only the ranges of parameter deviation are known.

4-6. A COMPARISON OF RATIONAL DESIGN METHODS FOR A PROCESS INVOLVING PARAMETER UNCERTAINTY

Several methods for the rational design of processes involving parameter uncertainties are classified from the viewpoints of the property of parameter uncertainties and design calculation. The general characteristics of these methods are compared with each other. These characteristics are made clearer by some numerical examples. From these discussions, the method which has been proposed by the author is shown to be more practical and simple for the rational design of processes involving uncertain parameters.

We consider the same problems as appeared in 4-2, that is, the static optimal design of a complex system composed of N subsystems as shown in Fig.4.1. This system equations are given by Eq.(4.1)-(4.3) and performance index is given by Eq.(4.4). Now it is assumed for convenience that the fixed or objective values of t numbers of output Y_i are given as D_i which is l_i dimensional vector. That is,

$$Y_i = D_i, \quad i=1,2,\dots,t \quad (4.49)$$

where

$$0 \leq t \leq N, \quad \sum_{i=1}^t l_i < \sum_{i=1}^N r_i.$$

This assumption is not essential and mathematical treatment is almost the same as one in 4-2.

The effect of small variations of the system parameter on the system outputs to be fixed is easily evaluated by using the adjoint system with the boundary conditions defined in Eq.(4.16)-(4.18).

When only the parameter P_i deviates, ΔY_n can be calculated by letting $\Delta M_i = 0 (i=1, \dots, N)$ in Eq. (4.19).

4-6-1 Various Rational Design Methods Taking into Account Parameter Uncertainty

[A]. *Various Rational Design Methods*

Recently, some methods for determining rationally the value of design variables or for estimating the design margin accounting for parameter uncertainty have been studied^{[4-1]~[4-5], [4-23]~[4-25]}. Most of those apply sensitivity analysis.

When dividing these methods from calculation procedure, two divisions are considered. One termed the One-step Method, is used to determine the value of the design by considering parameter uncertainty from the beginning. The other, termed the Two-step Method, is used to determine the design margin to be added to the nominal optimum value which is designed based on nominal or mean values of uncertain parameters. The methods by Rudd^[4-1] and Rohrel^[4-2] are included in the One-step Method, and the ones by Takamatsu^[4-5] are considered of the Two-step Method type.

In turn when dividing these procedures from the amount of information of parameter uncertainty, three divisions result. One is when only the nominal value of the parameter is known. The second class is when nominal value of the parameter and the range of the parameter deviation are known. And the third class is when the probabilistic density function of the parameter deviation is known. The information of the third class is the most extensive of the three.

As described above, rational design methods accounting for parameter uncertainty are classified. The comparison now follows:

(1) Method I

This method uses only the expected or nominal value $\bar{P}_i$. By it the design variable M_i is determined so as to minimize the objective function J when some given function composed of a parameter sensitivity coefficient of output vector Y_n ($n=1,2,\dots,t$) with respect to parameter deviation is held within some value. That is, M_i is determined by solving Eqs. (4.1)~(4.3), (4.49), (4.50) and (4.51)

$$S\left(\frac{\partial Y_1}{\partial P_1}, \dots, \frac{\partial Y_1}{\partial P_N}, \frac{\partial Y_2}{\partial P_1}, \dots, \frac{\partial Y_t}{\partial P_N}\right) \Big|_{\bar{P}_i} \leq g \quad (4.50)$$

$$\min_{M_i} \{J = \sum_{i=1}^N f_i(X_i, M_i)\} \Big|_{\bar{P}_i} \quad (4.51)$$

where g and S are the given matrix and matrix function, and it is assumed that a solution to M_i exists at least which satisfies Eqs. (4.1)~(4.3), (4.49) and (4.50). The value of $\frac{\partial Y_i}{\partial P_i}$ ($i=1,2,\dots,N$) is calculated easily by using Eqs. (4.16)~(4.19). This method is a One-step Method because the design value of parameters $\bar{P}_i$ is used only for parameter uncertainty. Moreover, by this method, controlling the undesirable deviation of the output vector is the first principle, while minimizing the objective function J is the second.

(2) Method II

Unlike Method I, Method II does the opposite, minimizing the objective function J as the first principle and controlling the undesirable deviation of the output vector as the second. That is, the design variable M_i is determined so as to minimize some given function composed of the parameter sensitivity coefficient of the

output vector Y_n when the original objective function is held under the value of $(1+\alpha) \times \bar{J}_{opt}$ where $\bar{J}_{opt}$ is the value of minimum J in Eq. (4.4) based on the nominal parameter value $\bar{P}_i$ subjected to Eqs. (4.1)~(4.3) and (4.49). When represented by equations,

$$\sum_{i=1}^N f_i(X_i, M_i) \frac{1}{P_i} \leq J_{opt} (1+\alpha) \quad (4.52)$$

$$\min_{M_i} \{ w_1^T S \left(\frac{\partial Y_1}{\partial P_1}, \dots, \frac{\partial Y_1}{\partial P_N}, \frac{\partial Y_2}{\partial P_1}, \dots, \frac{\partial Y_t}{\partial P_N} \right) w_2 \} \Big|_{P_i} \quad (4.53)$$

M_i is determined by solving Eqs. (4.1)~(4.3), (4.49), (4.52) and (4.53) where α is a constant giving the allowable amount of increase of the value of the objective function, and w_1, w_2 is the weighting vector. This method is a Two-step Method because $\bar{J}_{opt}$ must be calculated beforehand, and the nominal value of the parameter is used only for parameter uncertainty.

(1)' Method I' [4-25]

$$\min_{M_i} \{ J + w^T S \left(\frac{\partial Y_1}{\partial P_1}, \dots, \frac{\partial Y_1}{\partial P_N}, \frac{\partial Y_2}{\partial P_1}, \dots, \frac{\partial Y_t}{\partial P_N} \right) w \} \Big|_{P_i} \quad (4.54)$$

Method I and Method II are more practical than Method I' because it is difficult to give the weighting coefficient w quantitatively in spite of the fact that calculations by Method I or Method II are more difficult. Method I' is included here under Method I because Method I and Method I' are both One-step Methods.

(3) Method III [4-2]

This method uses the information of the range of the parameter deviation ΔP_i .

Let $J(M_{opt}, P)$ be the value of the objective function which

is the minimum value of J based on some parameter value P_i subjected to Eqs. (4.1)-(4.3) and (4.49). And let $J(M, P)$ be the value of the objective function based on P_i and some non-optimal value of design variable, M_i . Then we derive the relative sensitivity of the objective function, $S(M, P)$ by Eq. (4.55).

$$S(M, P) = \frac{J(M, P) - J(M_{\text{opt}}, P)}{J(M_{\text{opt}}, P)} \quad (4.55)$$

where

$$J(M_{\text{opt}}, P) = \min_M \{J(M, P)\} \quad (4.56)$$

Design variable M_i is determined so as to minimize the maximum value of relative sensitivity in the range of parameter deviation. That is, M_i is determined by solving Eqs. (4.1)~(4.3), (4.49), (4.57) and (4.58),

$$-\Delta P_i \leq P_i - \bar{P}_i \leq \Delta P_i \quad (4.57)$$

$$\min_{M_i} \{ \max_{P_i} \{ S(M, P) \} \} \quad (4.58)$$

where ΔP_i is a given constant vector.

This method means that the worst case of parameter deviation in a given situation is focused, and the performance index of the original design problem is weighed. In addition, if it is desired that the deviation of the output vector be small, M_i may be determined by solving Eqs. (4.1)~(4.3), (4.49), (4.57) and (4.59)

$$\begin{aligned} & \text{Min}_{\{M_i\} \{P_i\}} \{ \text{Max}\{S(M,P) + w_1^T \\ & \times S(\frac{\partial Y_1}{\partial P_1}, \dots, \frac{\partial Y_1}{\partial P_N}, \frac{\partial Y_2}{\partial P_1}, \dots, \frac{\partial Y_t}{\partial P_N}) w_2\} \} \end{aligned} \quad (4.59)$$

Method III is a One step-Method.

(4) Method IV^[4-5]

When the nominal value and the range of deviation of the parameter are given, we determine design variables by a Two-step Method. That is, the nominal optimal design value is once determined based on nominal values and next, the design margin to be added to nominal optimal design value is determined accounting for parameter uncertainty. Design margin ΔM_i is determined so as to minimize some objective function h , constructed by ΔM_i when ΔY_n is in the allowable range. That is, ΔM_i is determined based on Eqs. (4.60) and (4.61),

$$\begin{aligned} -C_{L,n} \leq \Delta Y_n \leq C_{U,n} , \quad \Delta M_m \geq 0 , \quad n=1,2,\dots,t \\ m=1,2,\dots,N \end{aligned} \quad (4.60)$$

$$P_i^k = \pm \eta_i^k \quad k=1,2,\dots,p_i$$

$$\text{Min}_{M_i} \{h(\Delta M_1, \dots, \Delta M_N)\} \quad (4.61)$$

and final value of design variable becomes $\bar{M}_i + \Delta M_i$.

Where $C_{L,n}$ and $C_{U,n}$ are given constant vectors, and the meaning of $\Delta P_i^k = \pm \eta_i^k$ is as follows: The sign of ΔP_i^k which is a component of ΔP_i should be chosen so that if the deviation ΔP_i^k causes a worse effect on ΔY_n . ΔY_n in Eq. (4.60), it can be calculated as a linear

function of ΔP_i and ΔM_i by using Eqs.(4.16)-(4.19). The design margin problem can be reduced to a linear programming program if in Eq.(4.61) is a linear function of ΔM_i . The calculation becomes very easy because of the adjoint system described by Eqs.(4.16)~(4.18). This method is a Two-step Method.

(5) Method V^[4-1]

Design variable M_i is determined so as to minimize the expected value of the objective function J with respect to P^i when the probability density function P^i is given. That is

$$\text{Min}_{M_i, P^i} \{ E [J = \sum_{i=1}^N f_i(X_i, M_i)] \} \quad (4.62)$$

M_i is determined by solving Eqs.(4.1)~(4.3), (4.49) and Eq.(4.62), where $E[]$ represents the expected value. This method is a One-step Method, and the calculation to solve Eqs.(4.1)~(4.3), (4.49) and Eq.(4.62) may be an usually complex if parameters are nonlinearly included in Eqs.(4.1), (4.2) or the system dimensions become larger.

(6) Method VI^[4-26]

Another method when the probability density function of ΔP_i is known is given as follows as an extension of Method IV using stochastic programming. This method was already proposed previously along with a precise explanation, so we will only explain it again briefly. The design margin ΔM_i is determined by solving Eqs.(4.63) and (4.64),

$$\begin{aligned}
\Delta Y_i + y_{i1} - y_{i2} &= C_{L,i} \\
\Delta Y_i + y_{i3} - y_{i4} &= C_{U,i} \\
y_{ij} &\geq 0, \quad \Delta M_m \geq 0 \\
i &= 1, 2, \dots, t, \quad j = 1, 2, \dots, 4, \quad m = 1, 2, \dots, N
\end{aligned} \tag{4.63}$$

$$\begin{aligned}
\text{Min } \{ & E [h(\Delta M_1, \dots, \Delta M_N) + \sum_{i=1}^t (E_{i1}^T y_{i1} + E_{i4}^T y_{i4})] \} \\
\{ \Delta M_i \} & \{ \Delta P_i \} \\
\{ y_{ij} \} &
\end{aligned} \tag{4.64}$$

where $y_{i1} \sim y_{i4}$ are slack variables which are introduced to equalize the inequality condition Eq.(4.60), and E_{i1}, E_{i4} are coefficients of penalty cost.

Now, if ΔM_i is determined by solving Eq.(4.63) and (4.64), the final design variables are given as $\bar{M}_i + \Delta M_i$. ΔY_i in Eq.(4.63) can be easily calculated by Eqs.(4.16)~(4.19) in the same way as Method IV. If h is the linear function of ΔM_i , ΔM_i is comparatively easily determined^[4-26].

[B]. Consideration of Various Methods

Table 4.4 shows the classification of these methods described above such as how according to parameter uncertainty utilization and if the method is of the one or two step type. Modified method may of course be considered because the various methods in Table 4.4 are only the typical ones.

It is difficult for us to theoretically compare and judge the general superiority of the various methods because the amount of information of parameter uncertainty really utilized in a method is different for each. For example, the nominal value $\bar{P}_i$ is only used in

Table 4.4 Rational design considering parameter uncertainty.

Computational Procedure	Known Properties of Parameter Uncertainty		
	Nominal Value $\bar{P}_i$	Nominal Value $\bar{P}_i$, Range of ΔP_i	Distribution of P_i
1-Step Method	(1) Method-I	(3) Method-III	(5) Method-V
2-Step Method	(2) Method-II	(4) Method-IV	(6) Method-VI

Method I and II. The nominal value $\bar{P}_i$ and the range of parameter deviation are used in Method II and IV, and the probability density function $\bar{P}_i$ or ΔP_i is used in Method V and VI.

In general, Methods V & VI may be more rational because the amount of the information of parameter uncertainty used in them is more plentiful. It's not always desirable to use these methods, however, from the viewpoint of the demand for exactness of the performance index, deviation of output variable, and amount of calculation needed to determine design variables. For example, if we want to hold the deviation of an output variable within a narrow range but will allow the increase of performance index J to some extent, Method II is more preferable for determining design variable M_i . If the probability density function is known but we want to calculate M_i as easily as possible, Method IV is selected. These methods are difficult to compare directly, as stated before, but we will point out, compare and discuss their general characteristics.

(1) Method II, Method III and Method V are mainly weighed on the basis of the original objective function of the nominal static optimal design. On the other hand, the other methods especially Method IV and Method VI are weighed according to the original objective function and deviation of the output variable.

(2) Satisfying Eqs.(4.1)-(4.3) and (4.49) with respect to P_i is a necessary condition for determining M_i by Method III and V. Then, it becomes clear from the number of independent variables that if $\sum_{i=1}^t l_i$ design variables are not changeable variables such as the tank volume of the reactor, control

system cannot be constructed. Moreover, it may be happen that the parameter deviation is not observable and that the time required for data analysis is too long to control. When some control system cannot be constructed as stated above, Method III and Method V cannot be used directly, and some modification is necessary.

(3) On the other hand, when $(\sum_{i=1}^t l_i)$ numbers of design variables M_i are operating variables, Method IV and Method VI must be modified to some extent. In reality, we must introduce the concept of the margin of operating variables, but it is still vague. Thus, the following modification is considered: $(\sum_{i=1}^t l_i)$ number of operating variables are taken as the same value as the nominal optimal design, and the design margins are evaluated with respect to the other design variables.

(4) As the design margin problem of Method III and VI can be reduced to linear and stochastic programming problems, it is necessary to evaluate the design margin not for all design variables but only for some. In general, the number of design variables to be added to the design margin is at most equal to the number of the output variables to be fixed, $\sum_{i=1}^t l_i$.

(5) When we compare each method from the viewpoint of the difficulty of computation, the calculations done by Method I and II are not so easy because inequality constraints are included in both. On the other hand, the amount of calculation in Method III is much more because the objective function J must be calculated for every value of P_i and M_i . Calculations by Method V become very complex as the dimensions of their parameter or

system becomes larger. On the other hand, calculations by Method IV and VI are comparably easy. In fact the calculation by Method IV may be the easiest of these six methods because it can be reduced to a L. P. problem.

(6) The deviation of the output variable will be on the safe side by Method IV. This may be clear from the fact that the design margin ΔM_z of Method VI is equal to the one of Method IV when $E_{i1} \rightarrow \infty$ and $E_{i4} \rightarrow \infty$.

(7) When the objective function J is composed of only design variable M_z , Method-III and Method V become meaningless. This will be made clear in example 4-6-2.

As described above, the applicable design method depends on the amount of the utilizable information of parameter uncertainty. It may be said, however, that Method IV and VI are convenient methods because calculations are easy. They are compared in the following examples:

[C] *Rational Design of a Simple Chemical Tank Reactor*

We consider a simple static optimal design problem of a completely stirred tank reactor^[4-27]. The reaction is represented by $A \rightarrow R$. It is a first order irreversible reaction at a constant temperature. The process equation is given by

$$F_{AO}X_A = V \cdot k \cdot C_{AO}(1 - X_A) \quad (4.65)$$

where the raw material is a saturated solution of A (concentration $C_{AO} = 0.1 \text{ mol/l}$) and has the flow rate $F_{AO} [\text{mol/hr}]$. k is the reac-

tion rate constant[1/hr], V is the tank volume [L] and X_A is the conversion rate of A. With the product flow rate F_R is set at 100[mol/hr]. The equation

$$F_R = F_{A0} X_A = 100 \quad (4.66)$$

is satisfied. The problem is to design a tank reactor so as to minimize S_t in Eq.(4.67),

$$S_t = V\$_b + F_{A0}\$_a + F_{A0}(1 - X_A)\$_r, \quad (4.67)$$

where the first, second, and final term represent the construction cost per unit time, present material cost for recovery of unreacted raw material, respectively. $\$_b$, $\$_a$, $\$_r$ are taken as follows:

$$\begin{aligned} \$_b &= 0.01[\text{yen/hr}], & \$_a &= 0.5[\text{yen/mol}], \\ \$_r &= 0.125[\text{yen/mol}]. \end{aligned}$$

Here, the nominal value of parameter k is taken as $k=0.2[1/hr]$. The result of the nominal optimal design at $k=0.2$ is shown in the first row of Table 4.5.

The rational design variables are calculated by the above six method accounting for parameter uncertainty. We assume that the reaction rate constant k has a uniform distribution from 0.1 to 0.3. That is, the information using an expected value is 0.2 used for Method I and Method II. In Method III and IV, the expected value of k being 0.2 and range of deviation being 0.1~0.3 are used. In Method V and VI, the uniform distribution from 0.1 to 0.3 is used.

(1) Method I

The deviation of F_{AO} is within 15% according to 50% change of k , V and F_{AO} determined by solving Eqs.(4.65)~(4.69).

$$\left. \frac{dF_R}{dk} \right|_{k=0.2} \leq \frac{100 \cdot 0.15}{0.2 \cdot 0.5} = 150 \quad (4.68)$$

$$\left. \min_V \{S_t\} \right|_{k=0.2} \quad (4.69)$$

(2) Method II

V and F_{AO} are determine so as to hold the increase of the objective function from the nominal optimal value within 10% by using Eqs.(4.65)-(4.67), (4.70) and (4.71),

$$S_t|_{k=0.2} \leq S_t(V_{opt},k)|_{k=0.2} \times 1.1, \quad (4.70)$$

$$\left. \min_V \left\{ \frac{dF_R}{dk} \right\} \right|_{k=0.2}, \quad (4.71)$$

where $S_t(V_{opt},k)$ is the value of the performance index of the optimal design at parameter k .

(3) Method III

Tank volume V is determined by using Eqs.(4.65)~(4.67) and (4.73),

$$S_t(V_{opt},k) = \min_V \{S_t\} \quad (4.72)$$

$$\min_V \left\{ \max_{k=0.1 \sim 0.3} \left\{ \frac{S_t(V,k) - S_t(V_{opt},k)}{S_t(V_{opt},k)} \right\} \right\}, \quad (4.73)$$

where $S_t(V,k)$ represent the value of S_t in Eq.(4.67) at tank volume V and parameter k . Because Eqs.(4.65) and (4.66) must be satisfied,

F_{AO} is not constant but must be changed to correspond to the value of k .

(4) Method IV

The design margin ΔV is determined so as to hold F_R greater than 85[mol/hr] if k deviates, that is, by using Eqs.(4.74) and (4.75),

$$\Delta F_R \geq -15, \quad |\Delta k| \leq 0.1, \quad (4.74)$$

$$\begin{array}{l} \text{Min}\{\Delta V\} \\ \Delta V \end{array}$$

In Eq.(4.74), the relationship between ΔF_R , ΔV and Δk can be determined easily from Eqs.(4.64) and (4.66). As F_{AO} is operating variable, F_{AO} is taken as the value of nominal optimal design, $F_{AO} = 189.4$ from the discussion described above. Rational design value V is calculated as $V = \bar{V}_{opt} + \Delta V$.

(5) Method V

V is determined based on Eqs.(4.65)~(4.67) and (4.76),

$$\begin{array}{l} \text{Min}\{E[S_t]\} \\ V \quad k \end{array} \quad (4.76)$$

where E_k is the expected value. F_{AO} must also be operated for the value of k .

(6) Method VI

The coefficient of penalty cost, E_1 is taken as $E_1 = 10^4$. ΔV is determined from Eqs.(4.77) and (4.78),

$$\Delta F_R + y_1 - y_2 = -15 \quad (4.77)$$

$$\min_{\Delta V, \Delta k} \{ E(\Delta V + E_1 y_1) \} \quad , \quad (4.78)$$

where Δk is uniformly distributed from -0.1 to 0.1. In this case we consider $F_{AO} = 189.4$ the same as in Method IV.

Results of rational design by the various methods are shown in Table 4.5. The expected values of output F_{AO} and original objective function S_t in Eq.(4.67) are listed on the right side of Table 4.5 where k is assumed to be distributed uniformly from 0.1 to 0.3. F_{AO} by Method III and Method V must be operated, however the expected values of F_R and S_t are shown in Table 4.5 for comparison where F_{AO} is determined so as to satisfy Eqs. (4.65) and (4.66). From Table 4.5 the following becomes clear: The tank volume obtained by Method I is the largest one compared to these obtained by the other five methods, and about 58% margin is added to the nominal optimal design $\bar{V}_{opt}$ at the nominal value of the parameter $k = 0.2$. On the other hand, about 25% of F_{AO} is decreased. The design margin evaluated at tank volume V by Method VI is the smallest of these methods, and only about 7% margin is evaluated.

We compare the expected values of output F_R and the objective function S_t . If F_{AO} is operable against the value k and the operating cost is negligible, Method V gives the most preferable result.

Table 4.5 Rational design by various methods.

Method	Rational Design		Expected Value		
	V	F_{A_0}	$E(F_R)$	$E(S_I)$	In the case of $F_{A_0} = \text{const.}$
Nominal Optimum Design	10,590	189.4	98	212	
I	16,667	142.8 ($\omega=0.86$) (in Eq. (14))	98	244	
II	15,249	148.8	98	233	
III	13,500	to be controlled	100	186	$V=13,500$ $E(F_R)=92$ $F_{A_0}=158.7$ $E(S_I)=233$
IV	12,500	189.4	105	230	
V	12,900	to be controlled	100	179	$V=12,900$ $E(F_R)=98$ $F_{A_0}=163.5$ $E(S_I)=218$
VI	11,340	189.4	101	219	

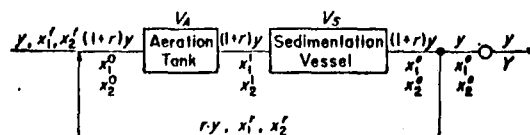
If F_{AO} is not operated, Method V gives the result of $E[F_R] = 98$, $E[S_t] = 218$ the same or a worse result than $E[F_R] = 101$, $E[S_t] = 219$ obtained by Method VI. Especially by Method III, $E[S_t]$ is the second minimum when F_{AO} is operated, while on the contrary, $E[S_t]$ is the fourth minimum when F_{AO} is not operated. When F_{AO} is not or cannot be operated, Method VI gives a good result from the viewpoint of $E[F_R]$ and $E[S_t]$ both being weighted.

Method I, II give a more complex result than the other methods because only the nominal values of the parameter are used. Method IV is the easiest for calculating design margin, more so than the other methods. Now we apply these methods to a more complex system design.

4-6-2 Rational Design of an Activated Sludge Process

[A] *Statement of The Problem*

We consider the static optimal design problem of a waste water treatment system using activated sludge. The system is composed of an aerator and sedimentation vessel as shown in Fig.4.4. BOD which represents quality of waste water and SS which represents the amount of microorganisms in the aerator and quality of waste effluent water are taken as state variables. This system can be considered as a system composed of a reactor and separator with recycle. Process equations are given as



- y : inlet waste flow rate [gal/hr]
 x_1^f : inlet waste BOD₅ [BOD ppm]
 x_2^f : inlet waste S.S. [SS ppm]
 r : return ratio
 V_A : volume of aeration tank [gal]
 V_S : volume of sedimentation vessel [gal]
 Y : total outlet BOD₅ [ppm]
 subscript 1 : BOD₅ [BOD ppm]
 2 : S. S. [SS ppm]
 superscript 0 : inlet of aeration tank
 1 : inlet of sedimentation vessel
 e : outlet of sedimentation vessel
 r : return sludge

Fig. 4.4 Waste treatment process.

follows from the literature^{[4.28],[4-29]}.

In the completely mixed aerator,

$$(1+r)y(x_i^0 - x_i^1) + V_A R_i = 0, \quad i=1,2 \quad (4.79)$$

where R_i represents reaction rate and is given by

$$R_1 = -kx_1^1 x_2^1 + \beta b x_2^1, \quad R_2 = a k x_1^1 - b x_2^1 \quad (4.80)$$

Parameters a , b , β and k are constants with respect to the reaction of microorganisms and are determined from experimental data.

Other nomenclature is explained in Fig.4.4.

In the sedimentation vessel, the following equations

$$x_2^e = 2 (x_2^1)^{0.5} \exp(-0.68 \frac{V_S}{(1+r)y}) \quad (4.81)$$

$$x_1^e = x_1^1$$

are satisfied. That is, it is assumed that BOD does not change in the sedimentation vessel and only SS does.

At the junction point of recycled activated sludge and input sewage, the following conditions

$$x_i^0 = \frac{x_i^f + r x_i^r}{1+r}, \quad i=1,2 \quad (4.82)$$

are satisfied. The water quality of effluent-treated waste water is measured as a total BOD Y as follows,

$$Y = x_1^e + mx_2^e \quad (4.83)$$

where m is the conversion coefficient from SS to BOD. Usually Y is given as a standard value of effluent treated water. Then, we consider the following static optimal design problem "to determine tank volumes V_A , V_S and return rate r so as to minimize J in Eq.(4.84) which is total volume under the given standard value of Y ",

$$J = V_A + V_S \quad (4.84)$$

In numerical calculation,

$$x_2^f = 0, \quad x_1^r = x_1^e \quad (4.85)$$

are used, and the values of parameters are given; $a=0.52$ [SSppm/BODppm], $b=0.005$ [l/hr], $k=0.0005$ [l/hr·SSppm], $\beta=0.7$ [BODppm/SSppm], $m=0.5$ [BOD/SSppm], $x_2^r=10^4$ [SSppm].

Input conditions are given as $y=2.5 \times 10^5$ [gal/hr], $x_1^f=260$ [BODppm].

From Eqs.(4.79)-(4.85), the following equations

$$\begin{aligned} y(x_1^f - x_1^1) + V_A(-kx_1^1x_2^1 + \beta bx_2^1) &= 0 \\ y\{rx_2^r - (1+r)x_2^1\} + V_A(akx_1^1x_2^1 - bx_2^1) &= 0 \\ x_2^e - 2(x_2^1)^{0.5} \exp(-0.681 \frac{V_S}{(1+r)y}) &= 0 \end{aligned} \quad (4.86)$$

are reduced.

Finally, the nominal static optimal design is used to determine V_A , V_S and r which minimize J in Eq.(4.84) under the conditions of process equation (4.86) and fixed output Eq.(4.87),

$$x_1^1 + mx_2^e = Y = C_{limit} = 30[\text{BODppm}] \quad . \quad (4.87)$$

In this case, it is not necessary to decompose the system into sub-systems in order to carry out the calculation.

Now the solution of nominal static optimum design is given as,

$$r = 0.8, \quad V_A = 1.575 \times 10^6 [\text{gal}], \quad V_S = 1.572 \times 10^6 [\text{gal}]$$

How large an effect each parameter deviation gives each state variable and output Y is shown in Table 4.6. In Table 4.6, some examples of normalized parameter sensitivity coefficient for each variable are shown. Normalization is made by multiplying the absolute value by parameter sensitivity coefficient. The normalized value means the deviation of variables, when parameters deviate by a relative percent. From Table 4.6, the deviations of input flow rate of waste water, y , input BOD x_1^f and reaction rate constant k gives a large effect to the output Y .

Now we consider the rational design of waste water treatment system accounting for parameter uncertainty. We assume that only the input flow rate y and BOD x_1^f have uncertainty because y and x_1^f have a great effect on output Y and because it is well known that

Table 4.6 Normalized parameter sensitivity.

State Variable x_i Parameter P_j	normalized parameter sensitivity $P_j \frac{dx_i}{dP_j}$			
	x_1^1	x_2^1	x_2^2	Y
y	1.55×10	3.55×10	2.95×10	3.03×10
x_1^f	1.70×10	6.96×10	9.78×10^{-2}	1.71×10
a	-5.35×10^{-1}	9.55	1.34×10^{-1}	-4.68×10^{-1}
b	6.73	-5.11×10	-7.18×10^{-2}	6.69
β	6.47	2.65×10	3.72×10^{-2}	6.49
k	-2.19×10	5.85	8.20×10^{-3}	-2.19×10

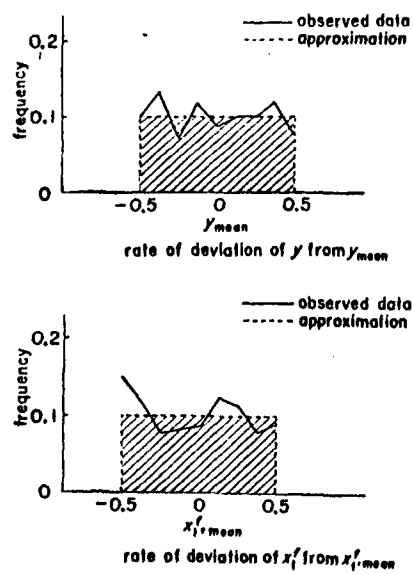


Fig. 4.5 Distribution of y and x_1^f .

the input flow rate and quality deviate or change hourly in a real sewage plant.

In such a sewage plant, both input flow rate and quality have a peak and the measurement of BOD x_1^f require 5days, but the average total retention time of the sewage plant is about 1day. Then, to consider the rational design of a sewage plant at construction, accounting for the uncertainty of y and x_1^f has practical value because of the control holding Y at the desired volume may be impossible.

Fig.4.5 shows an example of the deviation of y and x_1^f which was taken from three days real data at Kishoin Treatment Plant in Kyoto. From Fig.4.5, it may be natural to assume that both flow rate y and BOD x_1^f are distributed uniformly from -50% to 50% mean value. Next we consider the design of a waste water treatment plant taking into account the uniform distribution of y and x_1^f .

[B] Rational Design

Next we will do calculations by the six methods described above.

(1) Method-I

Considering that the deviation of out BOD Y is within 15ppm according to a 50% change of y and x_1^f , the design variables are determined by solving Eqs.(4.86)-(4.89),

$$y \cdot \frac{dY}{dy} + x_1^f \cdot \frac{dY}{dx_1^f} \bigg|_{\bar{y}, \bar{x}_1^f} \leq 30, \quad (4.88)$$

$$\min_{V_A, V_S, r} \{J = V_A + V_S\} \bigg|_{\bar{y}, \bar{x}_1^f}, \quad (4.89)$$

where $\bar{y}$, $\bar{x}_1^f$ are the nominal values of y and x_1^f and $\bar{y} = 2.5 \times 10^5$,
 $\bar{x}_1^f = 260$.

(2) Method II

Design variables are determined so as to minimize the deviation of output Y under the condition of the increase of the objective function being within 10% ($\alpha=0.1$), that is, by Eqs. (4.84)-(4.87), (4.90) and (4.91),

$$J \leq J(V_{A,opt}, V_{S,opt}, y, x_1^f) \Big|_{\bar{y}, \bar{x}_1^f} (1+\alpha) \quad , \quad (4.90)$$

$$\text{Min}_{V_A, V_S, r} \left\{ y \frac{dY}{dy} + x_1^f \frac{dY}{dx_1^f} \right\} \Big|_{\bar{y}, \bar{x}_1^f} \quad , \quad (4.91)$$

where $J(V_{A,opt}, V_{S,opt}, y, x_1^f)$ represent the value of the objective function of the original static optimum design at y and x_1^f .

(3) Method III

Rational designs are performed by using Eqs. (4.84)-(4.87), (4.92) and (4.93).

$$\text{Min}_{\{V_A, V_S, r\}} \left\{ \text{Max}_{y, x_1^f} \frac{(J(V_A, V_S, y, x_1^f) - J(V_{A,opt}, V_{S,opt}, y, x_1^f))}{J(V_{A,opt}, V_{S,opt}, y, x_1^f)} \right\} \quad , \quad (4.92)$$

$$\left| \frac{y - \bar{y}}{\bar{y}} \right| \leq 0.5 \quad , \quad \left| \frac{x_1^f - \bar{x}_1^f}{\bar{x}_1^f} \right| \leq 0.5 \quad (4.93)$$

where $J(V_A, V_S, y, x_1^f)$ is the value of J in Eq. (4.87) evaluated at V_A, V_S, y and x_1^f . $J(V_{A,opt}, V_{S,opt}, y, x_1^f)$ is a monotonously

increasing function with respect to y and x_1^f . V_A and V_S in Eq.(4.92) must satisfy Eqs.(4.86) and (4.87) at any point in the range of deviation of y and x_1^f . Then the following relation

$$J(V_A, V_S, y, x_1^f) = V_A + V_S \geq J(V_{A,opt}, V_{S,opt}, y, x_1^f) \quad \begin{matrix} y=1.5\bar{y} \\ x_1^f=1.5\bar{x}_1^f \end{matrix} \quad (4.94)$$

must be satisfied. As $J(V_A, V_S, y, x_1^f)$ does not depend on y, x_1^f under the condition of Eq.(4.94), the problem is to determine the minimum value of V_A and V_S which satisfies Eq.(4.94). That is, by Method III design variables are determined so as to minimize J in Eq.(4.84) under the conditions of Eq.(4.86) and (4.87), $x_1^f = 1.5 \cdot \bar{x}_1^f$ and $y = 1.5 \cdot \bar{y}$. This means that rational design is to solve the original problem at parameter values when parameter deviate to the greatest extent from the nominal value. If so, there may be no merit in using Method III in this case.

When the objective function is a function composed only of design variables, it is not necessary to treat those design variables as operating variables as explained in section 4-6-1. It can be seen that there is no advantage in this example by using Method III.

The sludge return ratio is assumed to be constant because the operation of r against the change of parameters may be difficult, in spite of the fact that r must be operated so as to satisfy Eq.(4.87). The value of r is taken as the optimal value of

r at $y = 1.5 \bar{y}$, $x_1^f = 1.5 \bar{x}_1^f$.

(4) Method IV

The design margins ΔV_A , ΔV_S are determined by using Eq. (4.95) so as to hold Y within the upper limit of 32[BODppm],

$$\Delta Y \leq 2, \quad |\Delta y| \leq 0.5 \bar{y}, \quad |\Delta x_1^f| \leq 0.5 \bar{x}_1^f \quad (4.95)$$

$$\text{Min}_{\Delta V_A, \Delta V_S} \{ \Delta V_A + \Delta V_S \}$$

The relationship between ΔY , Δy , Δx_1^f , ΔV_A and ΔV_S is given directly by Eq. (4.86) and partially by using Table 4.6. r is taken as constant in the same way as in Method IV. in spite of the fact that r may be considered as an operating variable. The value is taken as 0.8 which is the optimal value at the nominal parameter value.

(5) Method V

Design variables are determined by Eqs. (4.86), (4.87) and (4.96),

$$\text{Min}_{\{V_A, V_S, r\}} \{ E_{\{y, x_1^f\}} (J = V_A + V_S) \} \quad (4.96)$$

In this case V_A and V_S in Eq. (4.96) must also satisfy Eqs. (4.86) and (4.87) at any point in the range of deviation of y and x_1^f .

The situation is the same as in Method III, that is, rational design variables are calculated by solving the original problem at parameter values when the parameters deviate to the greatest extent from the nominal value. If so, then there may be no advantage given by using Method V in this problem. The design values are taken as the

same as in Method III.

(6) Method VI

The coefficient of penalty cost, E_4 is taken as $E_4 = 5 \times 10^5$. ΔV is determined from Eqs.(4.97) and (4.98),

$$\Delta Y + y_3 - y_4 = 2 \quad (4.97)$$

$$\text{Min}_{\{\Delta V_A, \Delta V_S\}} \{ E (\Delta V_A + \Delta V_S + E_4 y_4) \} \quad (4.98)$$

where $\Delta y/\bar{y}$, $\Delta x_1^f/\bar{x}_1^f$ deviate uniformly from 20.5 to 0.5, respectively. The sludge return ratio r is assumed to be a constant 0.8 in the same way as in Method IV.

The results of rational design by various methods are shown in Table 4.7. The expected value of the output total BOD Y are also listed when y and x_1^f distribute from $0.5\bar{y}$ to $1.5\bar{y}$ and from $0.5\bar{x}_1^f$ to $1.5\bar{x}_1^f$, respectively.

Moreover, the maximum and minimum values of the output total of BOD Y are calculated and listed as $Y_{\max}$ and $Y_{\min}$, respectively. The rate being over standard value of $Y (= 30 \text{ ppm})$ is represented by σ as shown in Table 4.7.

From Table 4.7, the following becomes clear. Total volume ($= J = V_A + V_S$) obtained by Method III or Method V, that is, the optimum value of J at $y = 1.5\bar{y}$, $x_1^f = 1.5\bar{x}_1^f$ is the greatest in the values obtained by the six methods, and about 80% margin is added to the nominal design. The total volume calculated by using Method II is the smallest, and V_A is over designed, while V_S is under designed in comparison with the nominal optimal design. This may

Table 4.7 Rational design by various methods.

Method	Rational Design				Expected Value			
	r	$V_A(\times 10^6)$	$V_S(\times 10^6)$	$J(\times 10^6)$	$E\{Y\}$	σ	$Y_{\max}$	$Y_{\min}$
Nominal Optimum Design	0.80	1,575	1,572	3,147	30.2	0.47	57.3	11.9
I	1.15	2,419	1,330	3,749	29.7	0.48	51.7	11.9
II	1.05	2,101	1,361	3,462	29.8	0.49	53.3	11.8
III	1.00	3,150	2,782	5,932	16.9	0	30.0	9.0
IV	0.80	3,765	1,572	5,337	20.8	0.10	37.0	9.5
V	1.00	3,150	2,782	5,932	16.9	0	30.0	9.0
VI	0.80	2,305	1,572	2,877	25.2	0.29	46.6	10.6

be explained by the given value of α . The design margin is added only to the sedimentation vessel when using Method IV and VI while a design margin is added both to the aeration tank and sedimentation vessel by the other methods. As stated in section 6-3-2, this reason comes from the fact that Method IV and Method VI apply L. P. or Stochastic programming.

The expected value of output Y computed by using Method I or II or the nominal optimum design does not differ from the fixed value, $30[\text{BODppm}]$. The values of $Y_{\max}$ and σ , however, are not small in calculations using Method I or II or nominal optimal design, and it becomes clear that the values of the design variables may not always be rational. While the rational values of the design variables in this example depend on the value of σ which means the ratio of Y being over the standard value, the design values resulting by using Method III or V may be excessive. If output Y is allowed to be over the standard value to some extent, the design using Method IV may give a good result. Moreover, the calculation of a design by Method IV may be the simplest.

4-7. CONCLUDING REMARKS

At first, a method for determining design margin, taking the known probability density function of parameter deviation into account for the plant design, has been proposed. This method is called a Two-step Method in this paper, which was used to estimate the design margin by considering parameter uncertainty after choosing nominal optimal design values based on nominal values of plant parameters. It will be simple and easy to calculate design margin by the method proposed here because it introduces adjoint variables with the help of stochastic programming. It became clear that the design margin to be evaluated when the probability density function of parameter deviation was known was less than that when the range of parameter deviation was known. The two numerical examples given in this paper showed this method to be more reasonable than the method utilizing only the ranges of parameter deviations.

Secondly, several methods for the rational design of processes involving parameter uncertainties are classified from the viewpoints of the property of parameter uncertainties and the procedure of design calculation. The general characteristics of these methods are compared with each other^[4-27]. These characteristics are made clearer by some numerical examples. From these discussions, the methods which have been proposed by the author are shown to be more practical and simple for the rational design of processes involving uncertain parameters.

NOMENCLATURE

- A_{ij} ; surface area of the heat exchanger [m^2]
 $C_{L,n}$; allowable lower limit of the deviation of output vector
 $C_{U,n}$; allowable upper limit of the deviation of output vector Y
 F_{A0} ; mole flow rate of fresh feed [mol/hr]
 M_i ; vector of design variable
 $\bar{M}_i$; nominal optimum value of M_i
 ΔM_i ; deviation of design variable from $\bar{M}_i$
 P_i ; column vector of parameter
 $\bar{P}_i$; nominal value of P_i
 ΔP_i ; deviation of parameter from $\bar{P}_i$
 R_i ; reaction rate
 S ; a function of sensitivity
 U_{ij} ; overall heat transfer coefficient [$Kcal/hr/m^2/^{\circ}C$]
 V ; tank volume [ℓ]
 X_i ; vector of state variable
 x_1^f ; BOD of input flow
 Y_i ; vector of sytem ouput variable
 y_{ij} ; slack variable
 y ; input flo rate [gal/hr]
 Z_i ; vector of i-th subsystem output to other subsystem
 α_i ; adjoint vector
 β_i ; adjoint vector
 γ_i ; adjoint vector
 η_{ij} ; coefficient of penalty cost

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CHAPTER 5

DESIGN MARGIN TAKING INTO ACCOUNT PARAMETER UNCERTAINTY - II

5-1. INTRODUCTORY REMARKS

In a usual process system design, a design margin or safety factor is added to or multiplied by the nominal design value in order to compensate for the undesirable effects of the many uncertainties included in the design procedure and system operation. Quantitative and rational evaluation of the design margin, however, has not been discussed sufficiently, especially for large complex process systems.

Others have proposed a method for estimating a quantitative design margin taking into account parameter uncertainty^{[5-4],[5-5]}. In this chapter, a method is developed for determining design margin in concert with manipulating variables. Since decision variables consist of design variables such as tank volume and manipulating variables such as recycle ratio, design margin may be determined rationally by considering movable ranges of the manipulating variables. The method proposed in this report is

simpler in calculation than other methods^{[5-2],[5-3]}, and also can result in some important information useful in the design procedure, for example, which manipulating variable strongly affects the output variables and performance index? At the end of this chapter, the design of a simple chemical reaction process with recycle is described as a numerical example of the proposed method.

5-2. DESIGN MARGIN IN CONCERT WITH CONTROL OF MANIPULATING VARUABLE

Description of problem

The system equations of a process system can be described by

$$f_1(x, u, M, P) = 0 \quad (5.1)$$

where, x, u, M, P, f_1 denote n -dim. vector of state variables, r -dim. vector of manipulating variables, m -dim. vector of design variables, p -dim. vector of parameters and n -dim. vector function, respectively. Output variables from the process l -dim. vector Z is given by

$$Z = f_2(x, u, M, P) \quad (5.2)$$

where f_2 represents l -dim. vector function ($l < r$).

The output vector Z is set at a certain specified values, C .

$$Z = C \quad (5.3)$$

where C is l -dim. constant vector. Nominal optimum design means that decision variables u and M are determined so that the value of a performance index J given by Eq. (5.4) takes the minimum value given a certain parameter value $\bar{P}$ and output value C .

$$J = g(x, u, M) \quad (5.4)$$

If the true value of parameter $\bar{P}$ is given beforehand, it may be enough for practical design to calculate the nominal optimum decision values $\bar{u}$, $\bar{M}$ based on the nominal parameter value $\bar{P}$.

The value of parameter P included in Eq. (5.1) and Eq. (5.2),

however, involve an inevitable error of estimation, and also frequently deviate from the nominal value $\bar{P}$ during an operating period. Usually, a design margin or a safety factor is added to or multiplied by the nominal design value for compensation of an undesirable deviation of the output variable or system performance caused by such parameter uncertainties. The problem investigated in this chapter is how to estimate a reasonable design margin ΔM which must be added to the nominal design value $\bar{M}$.

Determination of reasonable design margin

When a parameter deviates by ΔP from the nominal value $\bar{P}$, and decision variables u and M are also moved by Δu and ΔM respectively, from the nominal optimum values $\bar{u}$ and $\bar{M}$, the deviation of state variable Δx is given from Eq.(5.1) as follows,

$$\Delta x = -(\frac{\partial f_1}{\partial x})^{-1} \{ \frac{\partial f_1}{\partial u} \Delta u + \frac{\partial f_1}{\partial M} \Delta M + \frac{\partial f_1}{\partial P} \Delta P \} \quad (5.5)$$

where $\partial f_1 / \partial x$ represents a $n \times n$ nonsingular matrix and $\partial f_1 / \partial u$, $\partial f_1 / \partial M$, $\partial f_1 / \partial P$ represent $n \times r$, $n \times m$, $n \times p$ matrices, respectively. The superscript -1 indicates the inverse matrix. These matrices are evaluated at $\bar{P}$, $\bar{u}$, $\bar{M}$. Substituting Eq.(5.5) into the equation for a small perturbation of Eq.(5.2), the deviation of output vector ΔZ is given by the following equation,

$$\begin{aligned} \Delta Z = & \{ \frac{\partial f_2}{\partial u} - \frac{\partial f_2}{\partial x} (\frac{\partial f_1}{\partial x})^{-1} \frac{\partial f_1}{\partial u} \} \Delta u + \{ \frac{\partial f_2}{\partial M} - \frac{\partial f_2}{\partial x} \\ & (\frac{\partial f_1}{\partial x})^{-1} \frac{\partial f_1}{\partial M} \} \Delta M + \{ \frac{\partial f_2}{\partial P} - \frac{\partial f_2}{\partial x} (\frac{\partial f_1}{\partial x})^{-1} \frac{\partial f_1}{\partial P} \} \Delta P \end{aligned} \quad (5.6)$$

where $\partial f_2/\partial x$, $\partial f_2/\partial u$, $\partial f_2/\partial M$ and $\partial f_2/\partial P$ are $l \times n$, $l \times r$, $l \times m$, $l \times p$ matrices evaluated at $\bar{P}$, $\bar{u}$, $\bar{M}$, respectively. The range of parameter deviation ΔZ is assumed to be given by a p -dim. constant vector n from experience or experiments. Moreover, the allowable range of output deviation ΔZ is assumed to be given by $\Delta C_L \leq \Delta Z \leq \Delta C_U$, where ΔC_L and ΔC_U express the lower and the upper limits for an allowable range of ΔZ . Therefore the rational design margin can be determined based on the following relationship,

$$\min_{\Delta M, \Delta u} \{ \phi = \phi(\Delta M, \Delta u) \mid \Delta C_L \leq \Delta Z \leq \Delta C_U, \Delta M \geq 0, \Delta P_k = \pm \eta_k, \Delta u \in U \} \quad (5.7)$$

$k=1, 2, \dots, p$

where, U represents a domain of admissible control Δu , and ΔZ must be subjected to Eq.(5.6). The sign of ΔP_k which is a component of ΔP should be chosen so that the deviation of ΔP_k causes an undesirable effect on ΔZ_i . For example, consider that following equations can be written for Eq.(5.6),

$$\begin{aligned} \Delta Z_1 &= a_1 \Delta u + b_1 \Delta M + d_1 \Delta P_1 + e_1 \Delta P_2 \\ \Delta Z_2 &= a_2 \Delta u + b_2 \Delta M + d_2 \Delta P_1 + e_2 \Delta P_2 \end{aligned} \quad (5.6)'$$

and that the allowable ranges of ΔZ_1 and ΔZ_2 are given by

$$\begin{aligned} \Delta C_{L1} &\leq \Delta Z_1 \leq \Delta C_{U1} \\ \Delta C_{L2} &\leq \Delta Z_2 \leq \Delta C_{U2} \end{aligned} \quad (5.7)''$$

ΔC_L usually has a negative value, and moreover the constraint for ΔZ sometimes needs either the upper or the lower only bounded.

The sign of ΔP is uncertain, and it cannot generally be known whether ΔP is a negative or positive value. Only the absolute value of ΔP can be estimated. In some cases, it may be clear that P changes dynamically in one direction from the nominal value of $\bar{P}$.

Assuming that d_1 and e_1 take positive values and that ΔZ_1 must not be over the positive value of ΔC_{U1} , the sign of ΔP_1 or ΔP_2 must be positive. Assuming that d_2 and e_2 are negative and positive values, respectively and that ΔZ_2 must be greater than the negative value of ΔC_{L2} , the sign of ΔP_1 and ΔP_2 must be positive and negative, respectively. In practice ΔP_2 does not simultaneously have a positive value for ΔZ_1 and negative value for ΔZ_2 , but the above statement gives a result on the safe side.

In general, Φ represents a negative effect for adding some margins to the nominal design values. Here, Φ is defined as the first variation of the performance index J due to Δu and ΔM . The physical meaning of this definition is the determination of the margins of design and manipulating variables so that the deviation of J caused by ΔM and Δu becomes as small as possible. Then, Φ is defined by

$$\Phi = \left\{ \frac{\partial g}{\partial M} - \frac{\partial g}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial M} \right\} \Delta M + \left\{ \frac{\partial g}{\partial u} - \frac{\partial g}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial u} \right\} \Delta u \quad (5.8)$$

where $\partial g / \partial x$, $\partial g / \partial M$ and $\partial g / \partial u$ are n -dim., m -dim. and r -dim. row vectors evaluated at $\bar{u}$, $\bar{M}$ and $\bar{P}$. In Eq.(5.8) the coefficients multiplied by ΔM and Δu are not generally equal to zero. Eq.(5.7) subjected to Eq.(5.8) is reduced to a linear programming (L.P.) problem because Φ is a linear function of ΔM and Δu . Hereafter,

a solution of the L.P. problem is assumed to exist. The reasonable design margin ΔM may be determined from the solution of the L.P. problem given by Eqs.(5.6)~(5.8). The design margin obtained by this method (denoted by Method I) may be more rational than that obtained by the method proposed previously by the author and others^{[5-4],[5-5]} (denoted by Method II) because the manipulating variables to be movable in a certain specified range are considered. In fact, if the deviation Δu of a manipulating variable is sufficient to compensate for undesirable parameter uncertainties and also minimizes Φ , the addition of any design margin to the nominal design variable is not always necessary. Moreover, it is also shown from this consideration just which manipulating variable strongly influences the values of the output variable and performance index.

5-3. APPLICATION TO THE DESIGN OF A SIMPLE CHEMICAL REACTION PROCESS WITH RECYCLE

Nominal optimum design at steady state

Let us consider the design margin of a reactor in a simple chemical process with recycle shown in Fig.5.1 as an example of the method proposed in this chapter. The reactor is assumed to be a single C.S.T.R. with perfect mixing. The type of reaction is assumed to be Denbigh's reaction which is constituted of first order elementary reactions as shown in Fig.5.2. R is the desired product, and this is produced from the fresh feed containing only A (molar concentration C_{A0} [gmol/l]). The effluent flow from the reactor containing A , B , R , X and Y is assumed to be separated into a product flow containing only R , and the other flow containing A , B , X and Y . X and Y are the undesired products. A and B are partially recycled at the ratio of α to the amount of A and B in the inlet flow to the separator, and X and Y are also recycled at the ratio of β . Denoting the fraction of molar concentration C_i [gmol/l] of each component i to C_{A0} ($C_i = C_{A0} x_i$, $i=A,B,R,X,Y$) by x_i , the hourly molar flow rate of fresh feed by F_{A0} [mol/hr], the flow rate of the inlet flow into the reactor which consists of fresh feed and recycle flow by F_i [mol/hr] ((volumetric flow rate) $\times C_{A0} = F_i$), and the volume of the reactor by V , the process equations for a steady state are given by,

$$F_{A0} + \alpha F_i x_A - F_i x_A - V(k_B + k_X) C_{A0} x_A = 0$$

$$\alpha F_i x_B - F_i x_B + V C_{A0} \{k_B x_A - (k_R + k_Y) x_B\} = 0$$

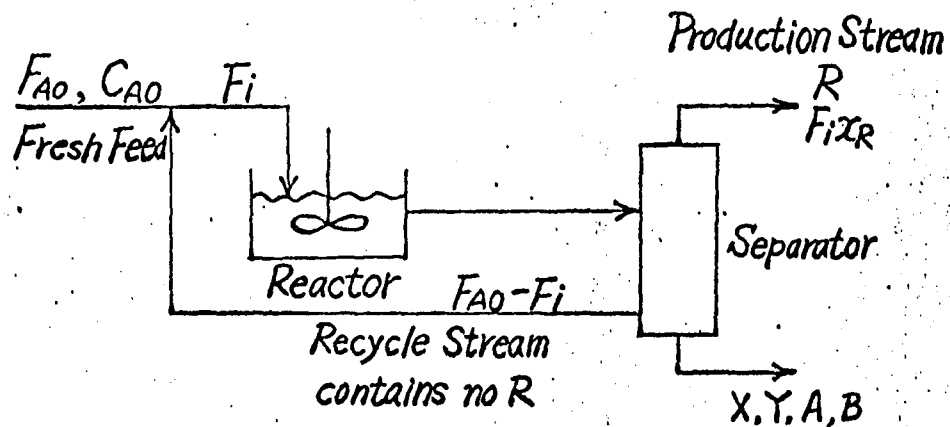


Fig. 5.1 A simple chemical reaction with recycle.

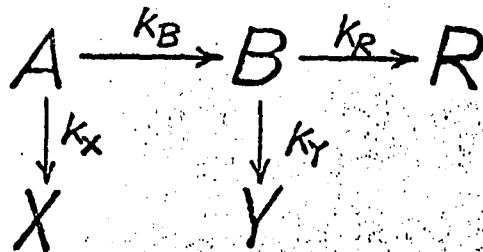


Fig. 5.2 Denbigh's reaction.

$$\begin{aligned}
\beta F_i x_X - F_i x_X + VC_{A0} k_X x_A &= 0 \\
\beta F_i x_Y - F_i x_Y + VC_{A0} k_Y x_B &= 0 \\
-F_i x_R + VC_{A0} k_R x_B &= 0 \\
x_A + x_B + x_R + x_X + x_Y &= 1
\end{aligned}
\tag{5.9}$$

where k_i ($i=B, R, X, Y$) [1/hr] shows the reaction rate constant for each elementary reaction. These equations correspond to Eq.(5.1) for a general expression.

Output states Z_1 and Z_2 are defined as

$$\begin{aligned}
Z_1 &= F_i x_R \\
Z_2 &= (x_X + x_Y) C_{A0}
\end{aligned}
\tag{5.10}$$

Z_1 is the amount of R produced hourly, and Z_2 is the molar concentration of undesired products X and Y . It is assumed that the value of Z_1 and Z_2 are desirably maintained as follows,

$$\begin{aligned}
Z_1 &= C_1 \\
Z_2 &= C_2
\end{aligned}
\tag{5.11}$$

Eqs.(5.10) and (5.11) correspond to Eqs.(5.2) and (5.3), respectively. For simplicity, the following objective function is assumed for the numerical calculation,

$$\begin{aligned}
J &= \left(\text{volume of reactor} \right) \left(\text{unit cost of reactor} \right) + \left\{ \left(\text{recycle rate of } A \text{ and } B \right) \right. \\
&\quad \left. + \left(\text{recycle rate of } X \text{ and } Y \right) \right\} \left(\text{unit cost for recycle} \right)
\end{aligned}$$

$$= V\$_b + \{\alpha F_i(x_A+x_B) + \beta F_i(x_X+x_Y)\}\$_r \quad (5.12)$$

Practical performance index J might be more complex, but the above simplification may be enough to illustrate a numerical example of a design margin problem. This form of J is referred to in the literature^[5-1]. The nominal optimum design is to determine the values of design variable V and operating variables α and β which minimize the value of performance index J given by Eq.(5.12), subjected to Eqs.(5.9), (5.10) and (5.11) under the specified values of F_{A0} , C_{A0} , C_1 and C_2 . The values of parameters and the boundary conditions used for the numerical calculation are given in Table 5.1. The result of the numerical calculation are shown in Table 5.2. The following can be recognized from the results : i) β is not equal to zero. Partial recycle of X and Y is more effective than no recycle of X and Y because the output molar concentration of X and Y , that is, Z_2 is specified. ii) The optimum recycle rate is 320[mol/hr] in this example, and the optimum retention time in the reactor is about 4[hr] based on C_{A0} .

Design margin for parameter uncertainty

For simplicity, the rate constants k_B and k_X are assumed to involve the maximum estimation error of $\eta^\circ[\%]$ for absolute values of the nominal values $\bar{k}_B$ and $\bar{k}_X$, respectively,

$$|\Delta k_B| \leq \frac{\eta^\circ}{100} \bar{k}_B, \quad |\Delta k_X| \leq \frac{\eta^\circ}{100} \bar{k}_X \quad (5.13)$$

Table 5.1 Given parameter values & boundary conditions.

$F_{A0}=100 \text{ mol/hr},$	$C_{A0}=0.1 \text{ mol/l},$	$k_B=0.4 \text{ hr}^{-1}$
$k_P=0.1 \text{ hr}^{-1},$	$k_X=0.02 \text{ hr}^{-1},$	$k_Y=0.01 \text{ hr}^{-1}$
$C_1=70 \text{ mol/hr},$	$C_2=0.005 \text{ mol/l},$	
$\$ _b=0.01 \text{ \$/l},$	$\$ _r=0.125 \text{ \$/mol/hr}$	

Table 5.2 Nominal optimum design.

$\bar{F}_i=320,$	$\bar{V}=1.27 \times 10^4,$	$\bar{\alpha}=0.921,$	$\bar{\beta}=0.278$
$\bar{x}_A=0.179,$	$\bar{x}_B=0.552,$	$\bar{x}_X=0.020,$	$\bar{x}_Y=0.030$
$\bar{x}_R=0.219,$	$\bar{J}=154 \text{ \$}$		

The value of η° is taken as 20 in this example. It is assumed that the allowable ranges for deviation of output variables Z_1 and Z_2 are given by

$$\Delta Z_1 \geq -\xi_1, \quad \xi_2 \geq \Delta Z_2 \geq -\xi_3 \quad (5.14)$$

The movable ranges of $\Delta\alpha$, $\Delta\beta$ (deviation of manipulating variables α and β) and ΔV (margin for design variable V) are constrained by

$$-\bar{\alpha} \leq \Delta\alpha \leq (1-\bar{\alpha}), \quad \bar{\beta} \leq \Delta\beta \leq (1-\bar{\beta}), \quad \Delta V \geq 0 \quad (5.15)$$

The design margin ΔV can be determined by solving the L.P. problem which is composed of Eqs.(5.6)~(5.8) and Eqs.(5.13)~(5.15). The result is shown in Table 5.3 for various allowable ranges of ΔZ_1 and ΔZ_2 . The design margins calculated by the method presented in the literature^[5-4] (Method II) which does not take into account the operation of manipulating variables, are also shown in the right column of Table 5.3. For Method II, design margin ΔV cannot compensate for undesirable deviation ΔZ_2 because the coefficient multiplied by ΔV in the equation of ΔZ_2 is positive, and ΔZ_2 is greater than ξ_2 even if ΔV is equal to zero. That is, by Method II, there is no feasible solution of the L.P. problem composed of Eqs.(5.6)~(5.8) and Eqs.(5.13)~(5.15). Thus design margin ΔV by Method II is determined so as to satisfy only the constraint ΔZ_1 .

From this calculated result the following is concluded.

1) Comparing the method proposed in this paper (Method I) with Method II, the design margin ΔV and the increment ΔJ of performance index J obtained by using Method I are smaller than those resulting from using Method II in each case except for case 1. For example,

Table 5.3 Rational design margin for parameter uncertainty.

allowable ranges of $\Delta Z_1, \Delta Z_2$				design margin						
				by the method proposed here				by the previous method		
case	ξ_1	ξ_2	ξ_3	ΔV	$\Delta \alpha$	$\Delta \beta$	ΔJ	ΔV	worst ΔZ_2	ΔJ
1	1.0	2×10^{-4}	10.75×10^{-4}	1097	-0.018	-0.278	1.26	565	7.94×10^{-4}	3.36
2	1.0	2×10^{-4}	20×10^{-4}	233	0.0022	-0.278	0.0095	"	"	"
3	1.0	2×10^{-4}	22.5×10^{-4}	0	0.0076	-0.278	-0.326	"	"	"
4	1.0	4×10^{-4}	20×10^{-4}	233	0.0022	-0.278	0.0095	"	"	"
5	1.5	2×10^{-4}	20×10^{-4}	150	-0.0008	-0.278	-1.01	365	6.68×10^{-4}	2.17

where $|\Delta k_B| \leq 0.08$, $|\Delta k_X| \leq 0.04$, $\Delta Z_1 \geq -\xi_1$, $\xi_2 \geq \Delta Z_2 \geq -\xi_3$.

in case 2, ΔV by Method I is 233[%] which corresponds to about 2[%] of the nominal value $\bar{V}$. On the other hand ΔV by Method II is 565[%] which corresponds to about 4.5[%] of the nominal value. ΔJ by Method II is about 350 times as much as that by Method I. In case 1, ΔJ by Method II is about 3 times of that by Method I, in spite of the fact that ΔV by Method II is smaller than that obtained by using Method I. Moreover, the deviation of output Z_2 due to the uncertainty of k_B , k_X cannot be compensated for by Method II, and the deviation ΔZ_2 is about 3 times of ξ_2 . These results suggest that Method I is more reasonable than Method II. ii) It becomes clear by comparing case 2 and 3 that manipulating variable β can sufficiently compensate for the effect of Δk_B and Δk_X so that ΔZ_2 is smaller than ξ_2 . It also becomes clear by comparing case 2 and 5 that the estimated design margin ΔV decreases if ξ_1 becomes smaller. iii) If ξ_3 is greater than or equal to 22.5×10^{-4} , the design margin ΔV is zero as shown in case 3. That is, α and β can sufficient controll ΔZ_2 within the specified allowable ranges of ΔZ_2 .

A method for determining rational design margin taking into account parameter uncertainty was developed for practical process system design^[5-6]. The design margin was determined by minimizing the deviation of a performance index under the allowable limitation of the deviation of output variables. An altered form of the performance index, however, may have to be discussed in the future. The method proposed here was applied to the design of a simple chemical reaction process with recycle. The numerical calculation explained that this method is more rational and practical.

NOMENCLATURE

- A ; reactant
- B ; intermediate product
- ΔC_L ; allowable lower limit of deviation of output vector
- ΔC_U ; allowable upper limit of deviation of output vector
- C_i ; molar concentration of the i th component ($i=A,B,R,X,Y$) [mol/L]
- F_{A0} ; mole flow rate of fresh feed [mol/hr]
- F_i ; output flow rate from reactor [mol/hr]
- k_i ; reaction rate constant [1/hr]
- M ; m-dim. column vector of design variable
- $\bar{M}$; nominal optimum value of M
- ΔM ; deviation of design variable from $\bar{M}$
- P ; p-dim. column vector of parameter
- $\bar{P}$; nominal value of P
- ΔP ; deviation of parameter from $\bar{P}$
- R ; desired product
- u ; r-dim. column vector of manipulating variable
- $\bar{u}$; nominal optimum value of u
- Δu ; deviation of u from $\bar{u}$
- V ; tank volume [L]
- $\bar{V}$; nominal optimum value of V [L]
- ΔV ; design margin of V [L]
- x_i ; mole fraction of each component i to C_{A0} [-]
- X ; undesired product
- Y ; undesired product
- α ; recycle ratio of A and B [-]
- β ; recycle ratio of X and Y [-]

ξ_i ; allowable upper or lower limit of output variable in Eq.(5.14)

η ; p-dim. vector of the range of parameter deviation

η^o ; relative range of parameter deviation in Eq.(5.13)

η_k ; k th element of vector η

$\$ _b$; hourly unit cost of reactor [\$/l/hr]

$\$ _r$; unit cost of recycle of A,B,X and Y [\$/mol]

superscript

-1 ; inverse matrix

subscript

A ; reactant

B ; intermediate product

R ; desired product

X ; undesired product

Y ; undesired product

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PART II

AN APPLICATION OF THE METHODOLOGIES TO WASTE WATER TREATMENT SYSTEM DESIGN

CHAPTER 6

INTRODUCTION TO DESIGN OF WASTE WATER TREATMENT SYSTEM

6-1. MODEL BUILDING IN A WASTE WATER TREATMENT SYSTEM

Over the past 50 years, extensive research has been conducted by universities, equipment manufacturers, and governmental agencies to delineate the physical, chemical and biological relationships which govern the operation of wastewater treatment processes. The literature on the performance of the individual processes is voluminous, but the techniques for calculating the performance of groups of processes working together as a system are limited. This is particularly true when the performance of the system as a whole is to be computed over a wide range of design and operating decisions associated with the individual processes. This part is an effort to bring together in one computational scheme the significant cost and performance relationships and to attempt to calculate the performance and cost of the system as a whole, based on relationships which have been developed for the processes individually.

Various researchers have proposed many mathematical models^{[6-1]~[6-9]}. Many of them are focused on the reaction model of the aeration tank,

and other simple models have also been proposed. Not many models of the other unit processes, for example, the final settler or thickener, have been proposed. Especially, simple models which represent the relations between output, input and design variables are not available yet. Recently, some studies on the simple model of each unit have been reported^{[6-6],[6-7]} and the study on the building of these models must be furthered.

If we want to discuss the design of a waste water treatment system, it is difficult for us to do so quantitatively because mathematical representations of the sludge treatment process are not yet sufficient.

When we want to design a waste water treatment system, we first build a mathematical model of the sludge treatment process because the process is not yet so represented. We choose the wet-air oxidation process as a sludge treatment unit and build a mathematical^{[6-10]~[6-14]} model of the process to be described in Chapters 7 and 8. The mathematical models of the other process of waste water treatment system are referred to in the literature^{[6-1]~[6-9]}.

6-2. OPTIMAL DESIGN OF A WASTE WATER TREATMENT SYSTEM

There have been studies on the optimal planning of a sewage treatment system^{[6-15]~[6-24]}, especially on the optimal design of a waste water treatment system^{[6-2],[6-25]}.

Many of them have been done with respect to the design of the aeration tank system^[6-2] or aeration-sedimentation tank system^{[6-9],[6-26]}. This is because it is generally difficult to build mathematical models of the other units. Recently, the representation of treatment or investment costs of the waste water treatment system have been given mathematically^{[6-27]~[6-30]}. Simulation studies of the design of waste water treatment^[6-5] has been done based on these economic and process models for each unit. We will design a waste water treatment system based on the model built here or referred to and apply some methods described in Part I to the design of this system with various uncertainty.

Some example in waste water treatment system design to which the theoretical considerations in Part I are applied have already been described in previous chapters, 4 and 5. We will not describe these examples once more here.

We will, however, explain the results of these new applications in the following chapters.

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CHAPTER 7.

SYSTEM IDENTIFICATION OF WET-AIR OXIDATION PROCESS-I THERMAL DECOMPOSITION

7-1. INTRODUCTORY REMARKS

With the advancement of waste treatment process it has been one of the most important problems how we treat the sludge. Up to now many methods for sludge treatment have been proposed, but roughly speaking, every process are constructed of three procedures of pre-treatment, dewatering and incineration. The differences between each process depend on how three procedures are devised and combined or under what principle these are developed. However, we have not yet determined the most effective way for various environmental conditions. The wet-air oxidation process that we are concerning is one of these sludge treatment processes.

The wet-air oxidation or Zimmerman process which is the subject of this paper, is a pressurized operation in which combustible matter dissolved or suspended in the water is oxidized by air at elevated temperatures and pressures^{[7-1]~[7-11]}. In these papers the effectiveness of the process is mainly discussed from the viewpoint of qualitative and practical considerations.

It is our purpose to identify the mathematical model of the reaction of this process and to obtain fundamental information for optimal control and optimal synthesis. We have performed many batch experiments on thermal decomposition and oxidation. In thermal decomposition the sludge is decomposed without oxygen, using equipment devised for this process. It is known that solid matter is decomposed into soluble matter in the thermal decomposition process as well as in the oxidation process. We propose a mathematical model of this thermal decomposition process which is expressed and identified by the state variables of COD and weight of solid matter, soluble non-evaporative matter and soluble evaporative matter in the sludge. The parameters of this mathematical model are estimated by a non-linear estimation technique.

7-2. STATE VARIABLES

Sludge consists of very complex compounds and this makes it difficult to represent the reaction of the thermal decomposition in a mathematical form. One way to represent the mathematical model would be to decompose the sludge into pure chemical species and to construct the model of elementary materials. However, because of the complexity and difficulty of this method, a more conventional method might be reasonable for process design and operation. From this viewpoint we represent the contents of the sludge by a general classification of its components and construct the mathematical model starting from this point. Four elements of the sludge are obtained by experiment and used in the classifications as follows.

- (1) solid matter (denoted by A).
- (2) soluble non-evaporative matter at 120°C (denoted by B)
- (3) soluble evaporative matter at 120°C (denoted by C)
- (4) pure water

Strictly speaking, the words evaporative or non-evaporative matter are not correct but they are used only in the sense mentioned below. The differentiation of solid matter from soluble matter may be correct for the purpose of this process and because of the fact that the COD values in both the solid and liquid change greatly during the process. There is no special need to divide the soluble matter into two groups, and this division was done because of the restriction of experimental technique rather than because of any physical significance. However, it might be expected that the soluble evaporative matter would contain the reaction products. Then, the

weight and COD of the solid matter (A), soluble non-evaporative matter (B), and soluble evaporative matter (C) are regarded as the state variables. The values of these state variables are measured by the following procedure.

Measurement of weight

The sample is centrifuged at 2000 rev./min for 5 min. The centrifuged sample is separated into the supernatant liquid and the rest by the inclination technique. The supernatant liquid is dried at a constant temperature of 120°C in the same way as the measurement of the total solids, and the weight of the residual substances is measured as the weight of soluble non-evaporative matter (B_{Wt}). The weight of total solid of the sample is measured at 120°C: the value is equal to the sum of the weight of solid matter (A'_{Wt}) and the weight of the soluble non-evaporative matter at 120°C (B_{Wt}). The weight of solid matter (A'_{Wt}) is given by subtraction of B_{Wt} from the weight of total solids ($A'_{Wt} + B_{Wt}$). The weight of the soluble evaporative matter (C_{Wt}) is calculated from the mass balance of A'_{Wt} , and B_{Wt} and C_{Wt} on the assumption that the value of C_{Wt} is negligible at the initial state of the reaction and that any matter other than solid matter, soluble non-evaporative matter and soluble evaporative matter is negligible and does not exist in the thermal decomposition. The value of C_{Wt} at any time of reaction can be obtained by subtracting the sum of the values of A'_{Wt} and B_{Wt} from the initial value of total solid. The measuring unit of these variables is mg/kg of total sludge.

Measurement of COD value

From the experimental considerations of COD test and several references [7-12],[7-13], the potassium dichromate method was chosen for the COD test and 2hr as the reflux time. The sample is first separated into solid and liquid phases by centrifuging. The COD value of the supernatant liquid is the sum of the COD value of the soluble non-evaporative matter (B_{COD}) and the COD value of the soluble evaporative matter (C_{COD}), and moreover the total COD of the sample is the sum of the COD value of the solid matter (A_{COD}), B_{COD} and C_{COD} . Therefore, A_{COD} is given by subtraction of the COD value of the supernatant liquid from the total COD. The residual substance arranged for the measurement of B_{Wt} is dissolved into pure water, and then the COD value of this dissolved sample is regarded as B_{COD} . Finally, C_{COD} is calculated by subtraction of B_{COD} from the COD value of the supernatant liquid. The unit of measurement of these variables is mg-COD/l total sludge.

The words of solid matter, soluble non-evaporative matter and soluble evaporative matter are used only for convenience, and the values of these substances are given experimentally, i.e., these variables are regulated by the experimental classification. When a complex compound is decomposed to some representative groups according to the experimental conditions, it is preferable that the conditions are not sensitive to quantitative expression in each group. In this connection the effect of centrifugal separation on the value of the quantitative expression was examined using frozen artificially cultured activated sludge. As a result of this examination, it was

shown that as an operating condition centrifugal separation is not sensitive. From this it was concluded that A'_{Wt} , B_{Wt} , C_{Wt} , A_{COD} , B_{COD} , and C_{COD} are reasonable as the state variables.

7-3. THERMAL DECOMPOSITION OF THE ACTIVATED SLUDGE

It is known that solid matter decomposes into soluble matter on wet-air oxidation^[7-2]. Our experiments show that the same phenomena also take place in thermal decomposition. Sludge was put into a magnetically stirred autoclave, with an inside temperature of 170°C 250°C and a pressure of 60~130kg/cm²-gage, without oxygen gas. During this batch process, the weight or the COD value of the solid matter greatly decreased, but the weight or the COD value of the soluble matter increased. This change is called thermal decomposition. For example, as shown in Fig.7.1, the values of A'_{Wt} , B_{Wt} , C_{Wt} , A_{COD} , B_{COD} , and C_{COD} widely change during this process, but the COD value of the total sludge hardly changes.

If we only want to decrease the weight of the solid matter for sludge treatment, it is sufficient for this purpose to treat the sludge by the thermal decomposition process. Actually, the process based on the principle of thermal decomposition is used for practical purposes. Moreover, since in the wet-air oxidation process, thermal decomposition is unavoidably included, it is necessary and meaningful to identify the mathematical model of the thermal decomposition process.

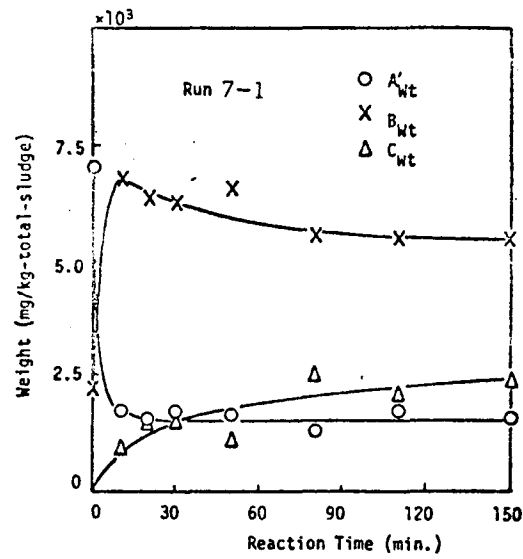


Fig. 7.1_a Change of weight vs. reaction time.

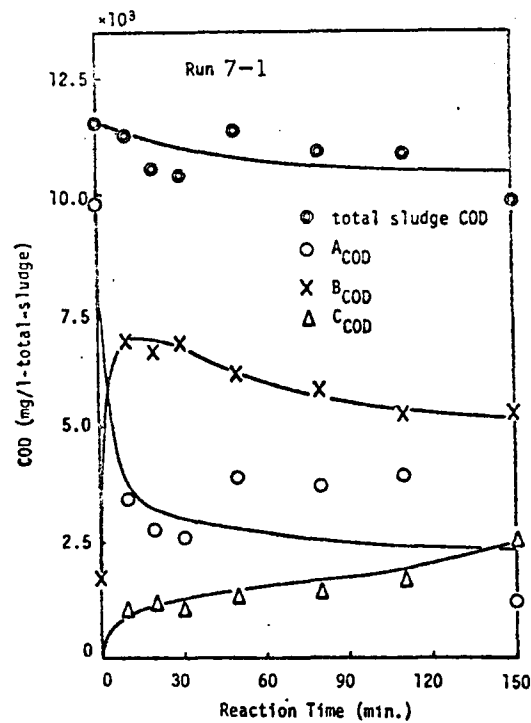


Fig. 7.1_b Change of COD vs. reaction time.

7-4. EXPERIMENT

To derive a mathematical model of the thermal decomposition process, we carried out experiments as follows.

Sample

The activated sludge used was grown from a feed of peptone, glucose, potassium chloride, sodium phosphate and manganese sulfate. It was concentrated by sedimentation, and frozen using dry-ice at about -60°C . From the analysis of the variance with respect to the experimental data, it was demonstrated that sludge preserved by this method is not influenced by the preservation time. The frozen activated sludge kept at a low temperature was used for the experiments.

Equipment

The equipment used for the thermal decomposition experiments is shown in Fig. 7.2. The volume of oil for the thermal medium, Kanecroll, is 50 l, at its temperature was held constant below 250°C . The reactor including the sample is a small autoclave and its volume is 16cm^3 . The needle valve is attached at the top of this reactor for pressurizing by nitrogen gas.

Procedure

The frozen sample was warmed and melted indirectly by warm water. The melted sample, 10cm^3 , was placed in the reactor and the inside of the reactor was pressurized using nitrogen gas. The free space in the reactor was filled only with nitrogen gas by displace-

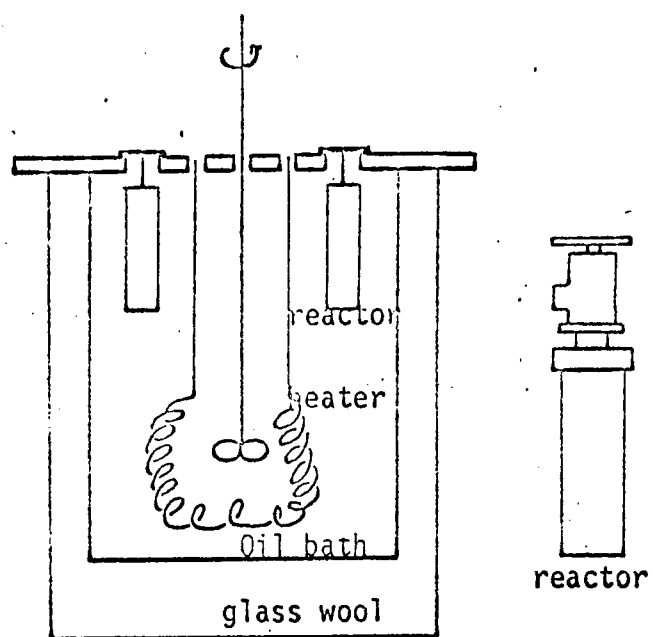


Fig. 7.2 Diagram of experimental equipment.

ment. The reactor was placed in the oil bath kept at a definite temperature as shown in Fig. 7.2. It may be removed at any time and cooled quickly in water. The weight and the COD values of this reacted sample are measured by the previously described method. The reaction temperature is measured in equipment similar to that in the reactor, which is also put in the oil bath, and by A-C thermocouple. The pressure of the reaction is calculated from the initial nitrogen gas pressure and the vapor pressure of water, assuming ideal conditions.

Measurement of state variables

The weight and COD values of A, B and C were measured by the method described. The initial value of suspended matter in the sample was measured as follows: The sludge was heated for 1 hr at 600°C, leaving fixed suspended matter. The weight of this residual substance is defined as the fixed suspended matter; it has the unit of mg/kg of total sludge. With our artificially cultured sludge adding ammonium carbonate had no effect on the value of the fixed suspended matter and this was omitted in our experiments. The necessity for measuring the initial value of the fixed suspended matter will be described later.

Experimental conditions

Three elements of initial concentration, temperature and pressure are considered as the conditions of the reaction. These conditions are shown in Table 7.1 & Fig. 7.3. The temperature and the pressure shown in Table 7.1 indicate the value which had become con-

stant, after several minutes from the start pointing of the reaction process, as shown in Fig.7.3. The fractions of the fixed suspended matter are also shown in Table 7.1.

Experimental results

The results of the experiments under the condition of nearly constant temperature are shown in Fig.7.1, Fig.7.4~Fig.7.9. The result of the experiment under the condition of unsteady temperature is shown in Fig.7.10. Each run number in these figures corresponds to that shown in Table 7.1, which gives the experimental data, and the solid curves show the calculated values obtained by the model described later. From these Figures, the following are recognized.

First, as shown in Fig.7.1, the weight of the solid matter (A'_{Wt}) decreased very quickly and tends to a steady value. This steady value ought to represent the weight of the solid that cannot be thermally decomposed. On the other hand, the value of the fixed suspended matter represents the fraction of the sludge that cannot be oxidized at 600°C, but since non-oxidizable matter may also not be decomposed in the thermal decomposition process, it may be concluded that this steady value is regarded as the value of the fixed suspended matter (denoted by A_{fs}). Therefore, in Figs.7.4 ~ 7.10, the weight of the solid matter (denoted by A'_{Wt}) shows the value of $A'_{Wt} - A_{fs}$.

Secondly, it is recognized that the weight of the soluble non-evaporative matter (B_{Wt}) increases very quickly and then decreases slowly, and finally reaches a certain value. It may be obvious from this fact that the soluble non-evaporative matter (B) is an inter-

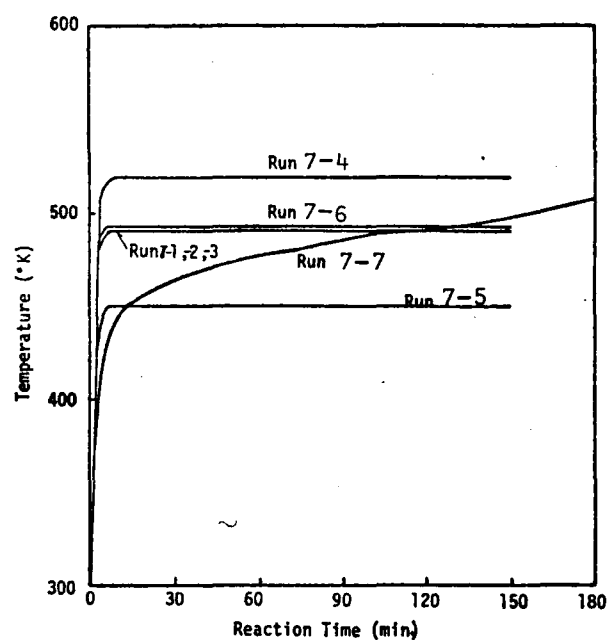


Fig. 7.3 Reaction temperature vs. reaction time.

Table 7.1 Conditions of the experiments.

Run No.	$A_{wt, \text{init.}}$ (mg/kg)	$A_{\text{COD, init.}}$ (mg/l)	Non-volatile (mg/kg)	Temp. (°K)	Pressure (kg/cm ²)
7-1	7080	9830	1150	490.5	66.7
7-2	15700	21830	2920	489.4	65.0
7-3	26220	30800	3740	490.5	66.7
7-4	7230	9620	1360	519.0	91.6
7-5	6450	10300	1090	450.0	49.0
7-6	6430	8800	1440	493.2	85.4
7-7	6680	9600	1240	FIG. 3	

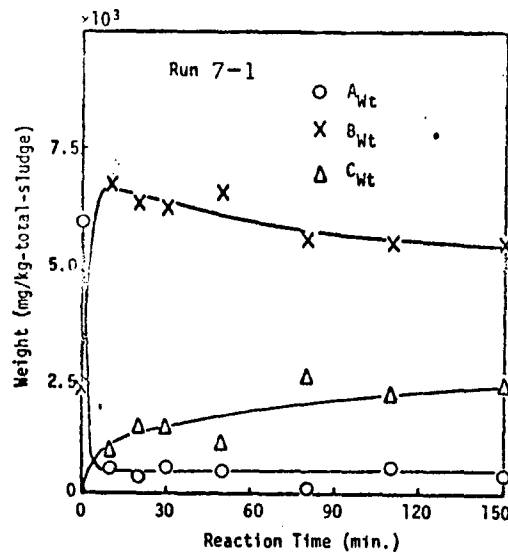


Fig. 7.4_a Change of weight vs. reaction time.

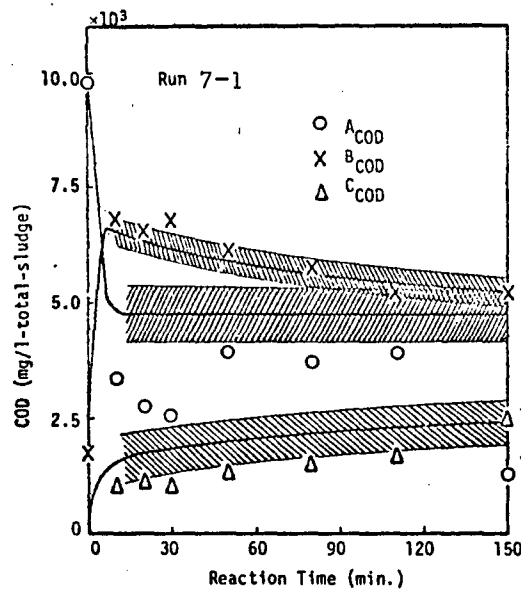


Fig. 7.4_b Change of weight vs. reaction time.

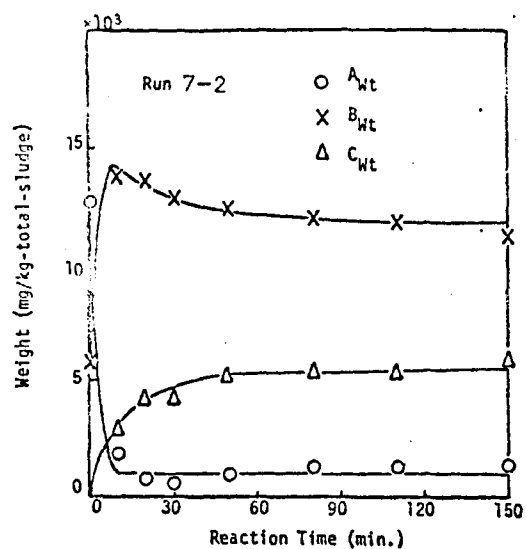


Fig. 7.5_a Change of weight vs. reaction time.

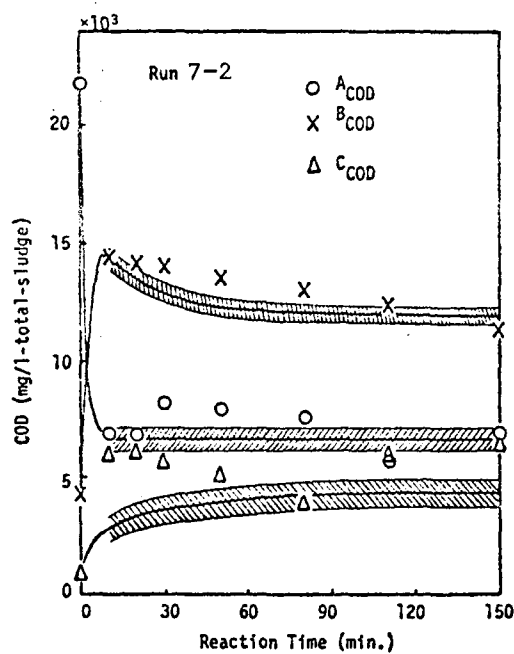


Fig. 7.5_b Change of COD vs. reaction time.

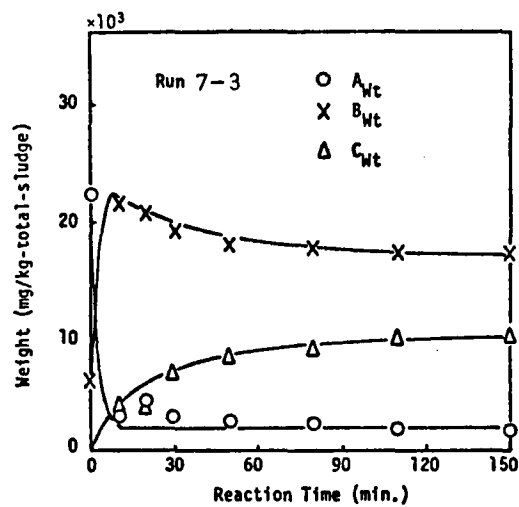


Fig. 7.6_a Change of weight vs. reaction time.

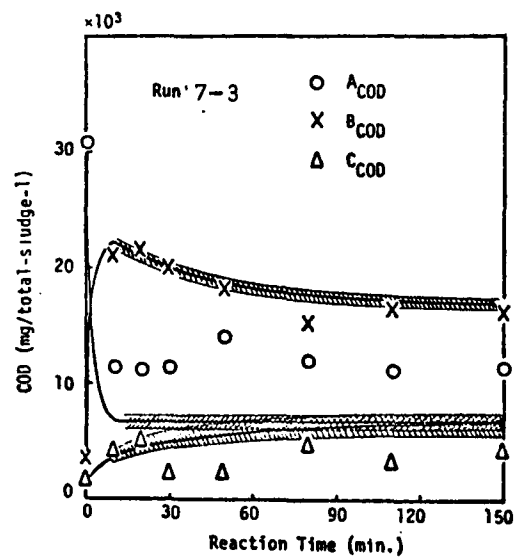


Fig. 7.6_b Change of COD vs. reaction time.

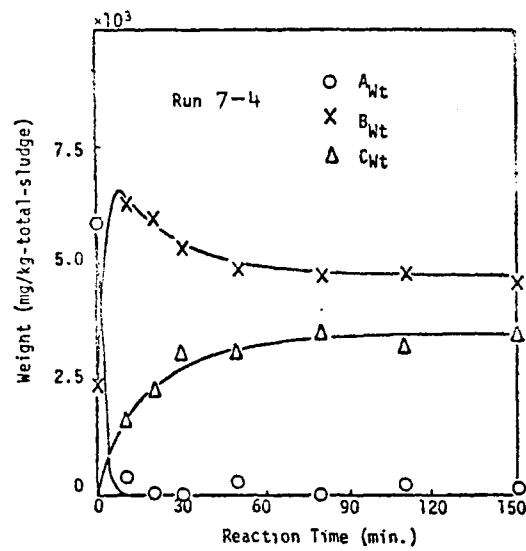


Fig. 7.7_a Change of weight vs. reaction time.

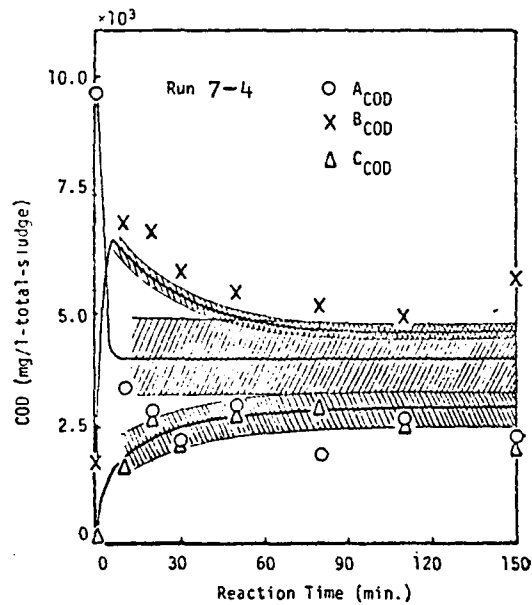


Fig. 7.7_b Change of COD vs. reaction time.

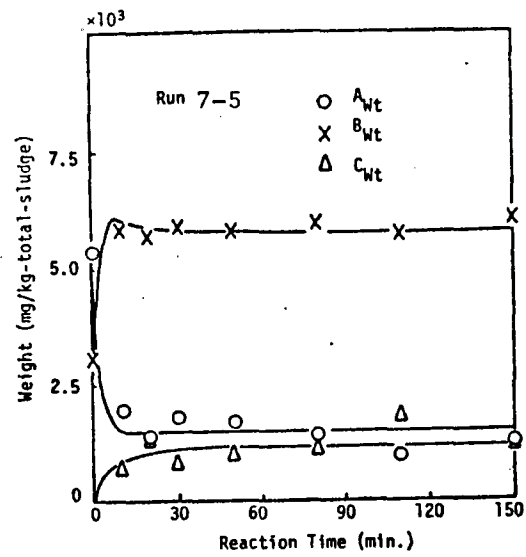


Fig. 7.8_a Change of weight vs. reaction time.

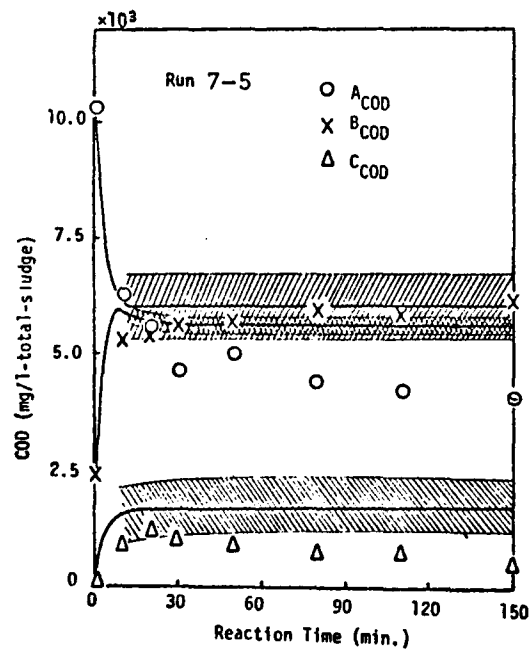


Fig. 7.8_b Change of COD vs. reaction time.

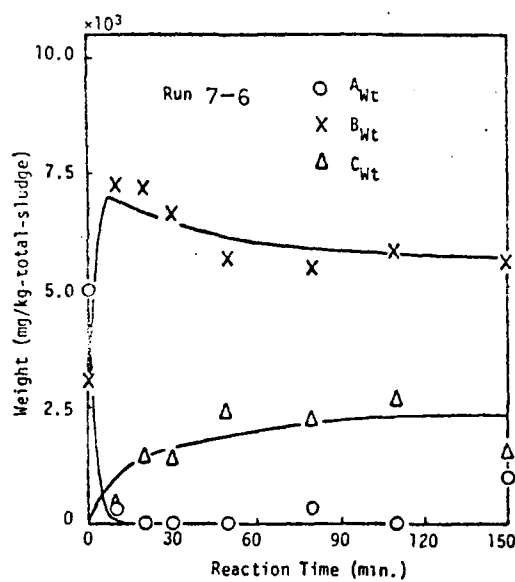


Fig. 7.9_a Change of weight vs. reaction time.

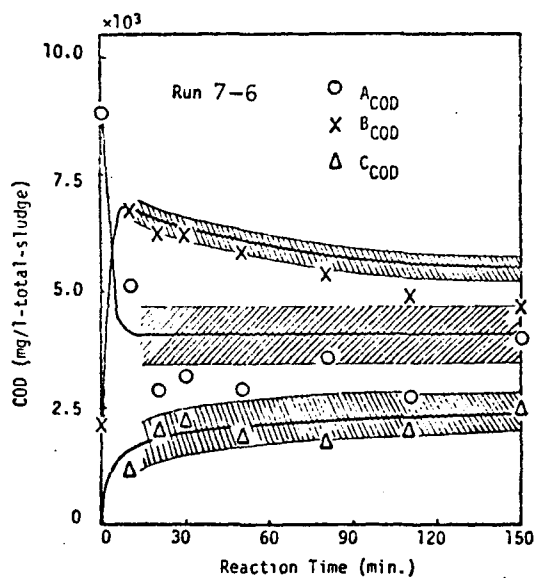


Fig. 7.9_b Change of COD vs. reaction time.

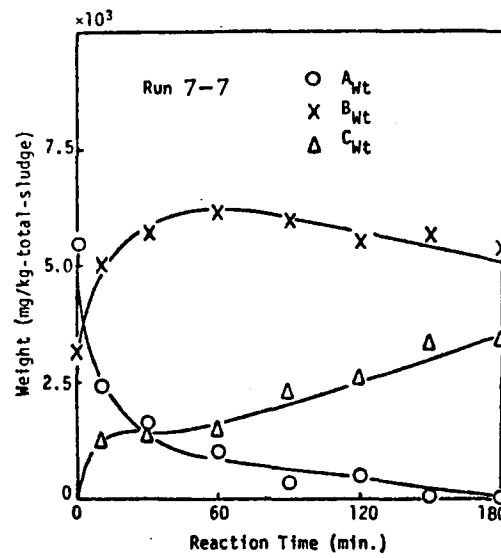


Fig. 7.10_a Change of weight vs. reaction time.

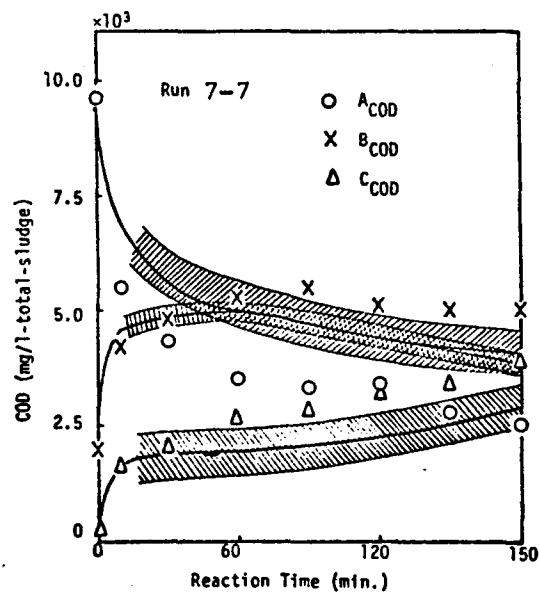


Fig. 7.10_b Change of COD vs. reaction time.

mediate product. However, as shown in Fig.7.8, there is also the case that a peak value of B_{Wt} does not exist. Therefore, it may be estimated that the reaction producing B apparently depends on the reaction temperature. On the other hand, the weight of the soluble evaporative matter (C_{Wt}) increases gradually and finally reaches a fixed value. The effect of the initial concentration is not clear at a glance of the shape of the change in state variables, but it will be discussed later.

Finally, the change of COD value is similar to the change of the weight with respect to the pattern of time response. Regarding the similarity in the shapes of the change of the weight and the COD, it is easily estimated that the COD value of each state variable may be related with the weight, i.e., the mathematical model based on the COD value will be related in the model by the weight, which state variables are A_{Wt} , B_{Wt} , and C_{Wt} .

7-5. MATHEMATICAL MODEL

As previously described, it may be meaningful to construct the model based on the weight of A_{Wt} , B_{Wt} and C_{Wt} independently of the COD, because the change of the component of sludge gives the change of the COD value and the weight of each variable represents grossly the component of the sludge. At first the model using the weight is discussed and next the model using the COD value.

Model of the thermal decomposition process with respect to the weight

As mentioned previously, it is assumed that A'_{Wt} doesn't react totally but partially. It may be natural to consider that the non-reacted part of A'_{Wt} is equal to the value of the fixed suspended matter ($A_{f.s.}$), but this idea is not directly accepted, because it is seen from the experimental data that A'_{Wt} does not converge to $A_{f.s.}$ even after a long reaction time. That is to say, $A_{Wt} - A_{f.s.}$ does not converge to zero. Plotting the ratio of the converged value of A_{Wt} to the initial value of A_{Wt} against the reaction temperature T , and recognizing that this ratio is the linear function of T , it may be said that the non-reacted part of A_{Wt} is the linear function of T .

Also with the soluble matter it is necessary to consider in more detail, i.e. it should be confirmed whether the initial soluble matter in the sample and the soluble matter produced from the solid matter are of the same class or not. Comparisons of the change of the initial soluble matter given by using the sample without A , and the usual one given from the experiment by the sample containing A ,

are shown in Fig.7.11. From this result it may be reasonable to assume that the initial soluble matter is the same as the soluble matter produced from the solid matter during reaction.

No matter except A,B and C exists during the thermal decomposition reaction. The model shown in Fig.7.12_a may then be of the most simple kind, including the reaction paths between each variable of A, B and C. The reaction paths from B to A and from C to A are physically meaningless, so that the model shown in Fig.7.12_a may be simplified as shown in Fig.7.12_b. The reaction order and the existence of each path in this model will now be discussed. At first, the effect of concentration is considered. Run 7-1, 7-2 which are rearranged by normalizing technique are shown in Fig.7.13; it is seen that the pattern of conversion of A_{Wt} is almost equal in both cases, and similarly with B_{Wt} . If all the reaction paths of this model are of the first order, the curves of the conversion on A_{Wt} and the yield on B_{Wt} do not, respectively, depend on the initial concentration. Therefore, all reaction paths in this model are approximately expressed in first order. Next to be discussed is whether each reaction path exists or not. From the shape of the time-response of B_{Wt} the reaction paths from A to B and from B to C are seen to exist. The existence of the other paths is considered, i.e., whether the reaction path from A to C exists or not, or whether the reaction is a parallel or series reaction. Here, the rate constants of each reaction path are denoted, respectively, by k_1, k_2, k_3 and k_4 , as shown in Fig.7.12_b. Because of each reaction being first order, the limited value of the ratio of C_{Wt} to $(B_{Wt} - B_{Wt,init.})$ when the time t approaches zero, is given as follows, for the case of parallel

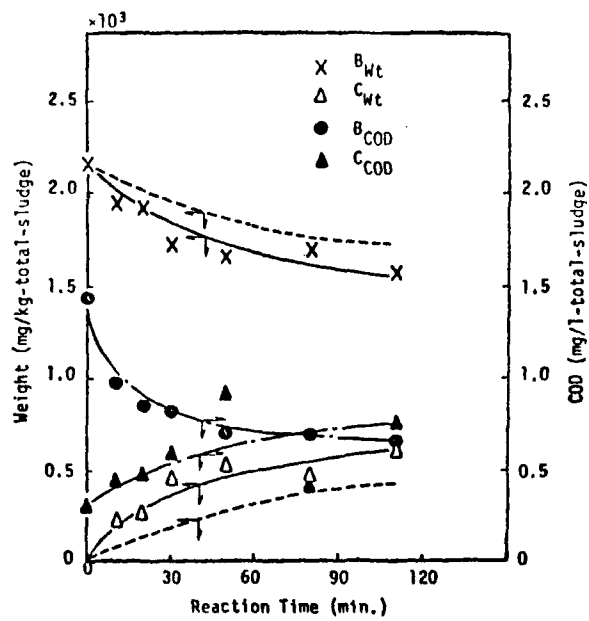


Fig. 7.11 Thermal decomposition of soluble matter.

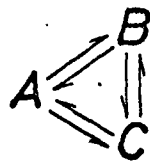


Fig. 7.12_a

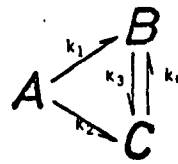


Fig. 7.12_b

Model of the thermal decomposition.

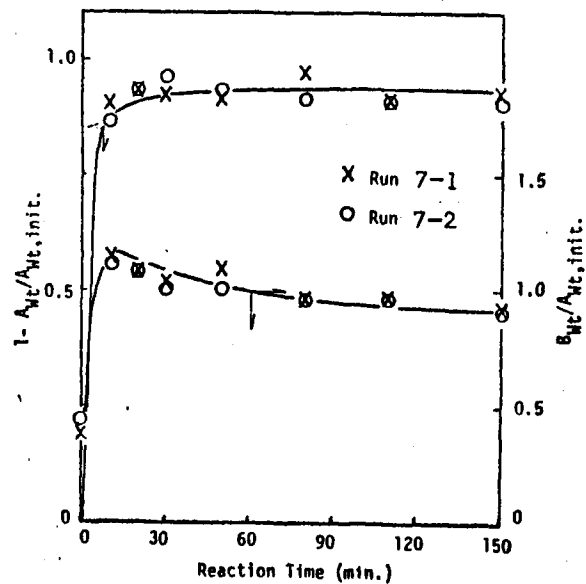


Fig. 7.13 Conversion and yield.

reaction

$$\lim_{t \rightarrow 0} \frac{C_{Wt}}{B_{Wt} - B_{Wt,init.}} = \frac{k_2 \cdot A_{Wt,init.} + k_3 \cdot B_{Wt,init.}}{k_1 \cdot A_{Wt,init.} - k_3 \cdot B_{Wt,init.}} \quad (7.1)$$

where $B_{Wt,init.}$ is the initial value of B_{Wt} and $C_{Wt,init.}$ is assumed to be equal to 0. For the case of series reaction, that is,

$$k_2 = 0,$$

$$\lim_{t \rightarrow 0} \frac{C_{Wt}}{B_{Wt} - B_{Wt,init.}} = \frac{k_3 \cdot B_{Wt,init.}}{k_1 \cdot A_{Wt,init.} - k_3 \cdot B_{Wt,init.}} \quad (7.2)$$

The equations (1) and (2) do not depend on whether the reaction path from C to B exists or not, for the $C_{Wt,init.}$ is equal to 0. If $B_{Wt,init.}$ is less than $A_{Wt,init.}$ and k_3 is much less than k_1 , the equations (1) and (2) are approximately rewritten as follows, for the case of the parallel reaction,

$$\lim_{t \rightarrow 0} \frac{C_{Wt}}{B_{Wt} - B_{Wt,init.}} \approx \frac{k_2}{k_1} \quad (7.3)$$

and for the case of series reaction,

$$\lim_{t \rightarrow 0} \frac{C_{Wt}}{B_{Wt} - B_{Wt,init.}} \approx 0 \quad (7.4)$$

when the data in Fig.6a are compared with the data in Fig.11, it will be seen that the above conditions with respect to the ratio of $B_{Wt,init.}$ to $A_{Wt,init.}$ and the ratio of k_3 to k_1 are satisfied. Therefore, the value of

$$\lim_{t \rightarrow 0} [C_{Wt} / (B_{Wt} - B_{Wt,init.})]$$

can be used to determine whether the reaction path from A to C exists or not. From the data in Fig.6a, the ratio of C_{Wt} to $(B_{Wt} - B_{Wt,init.})$

is plotted against time t , as shown in Fig.7.14. By extrapolation, it is seen that the value of

$$\lim_{t \rightarrow 0} [C_{Wt} / (B_{Wt} - B_{Wt,init.})]$$

is not equal to 0, and that the reaction path from A to C exists.

Moreover, $\frac{d^2 C_{Wt}}{dt^2}$ is convex for the case of parallel reaction, on the contrary $\frac{d^2 C_{Wt}}{dt^2}$ is concave for the case of series reaction. This leads the existence of the reaction path from A to C.

The existence of the reaction path from C to B is checked as follows.

It may appear strange that the reversible reaction exists in thermal decomposition. However, since the distinction between soluble non-evaporative matter and soluble evaporative matter depends only on the temperature in the vapor, it may not be unreasonable from the global viewpoint to consider that the reaction between B and C is reversible. If the reaction from C to B does not exist, the converged value of B_{Wt} cannot be conveniently explained. If the rate constant of the reaction is according to the Arrhenius type, the ratio of C_{Wt} to B_{Wt} at a steady state is a function of the temperature only, for the first order reaction. The plot of $\frac{1}{T}$ vs. the ratio of the converged value of C_{Wt} to the converged value of B_{Wt} becomes a straight line as shown in Fig.7.15. These converged values are taken from the data shown in Fig.7.4_a~Fig.7.10_a. From this result, the assumption that the reaction from C to B is reversible may be acceptable.

The conditions of pressure does not directly affect the thermal decomposition rate. This has already been reported for the wet-air oxidation process [7-1]. Consequently the effect of pressure is not considered.

Finally, on the assumption that the rate constant is of the Arrhenius type, the mathematical models of the thermal decomposition

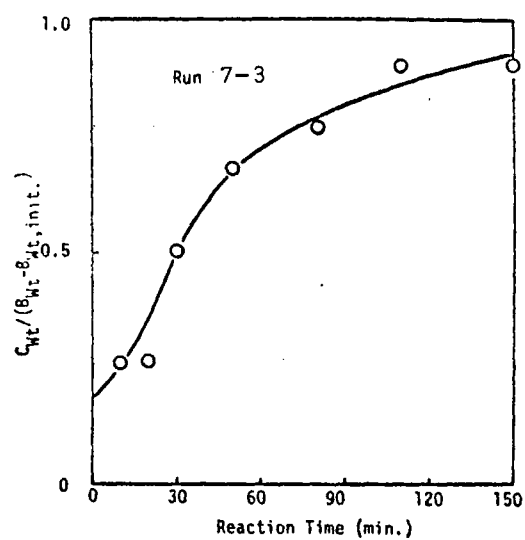


Fig. 7.14 $C_{Wt} / (B_{Wt} - B_{Wt,init})$.

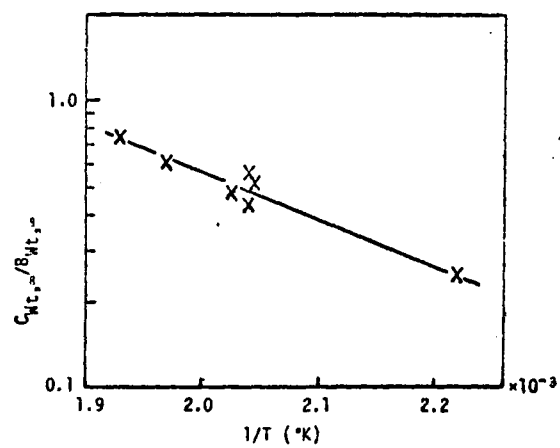


Fig. 7.15 $C_{Wt,\infty} / B_{Wt,\infty}$ vs. $1/T$.

process based on weight change become as follows

$$\frac{dA_{Wt}}{dt} = -(k_1 + k_2) \cdot (1 - \xi) \cdot A_{Wt} \quad , \quad (7.5)$$

$$\frac{dB_{Wt}}{dt} = k_1 \cdot (1 - \xi) \cdot A_{Wt} - k_3 \cdot B_{Wt} + k_4 \cdot C_{Wt} \quad , \quad (7.6)$$

$$C_{Wt} = A_{Wt,init.} + B_{Wt,init.} - A_{Wt} - B_{Wt} \quad , \quad (7.7)$$

where the initial conditions are

$$A_{Wt} \Big|_{t=0} = A_{Wt,init.} \quad , \quad B_{Wt} \Big|_{t=0} = B_{Wt,init.} \quad , \quad C_{Wt} \Big|_{t=0} = 0 \quad , \quad (7.8)$$

and k_1, k_2, k_3, k_4, ξ are

$$k_i = k_i^0 \cdot \exp\left(-\frac{E_i}{R \cdot T}\right) \quad , \quad i = 1, \dots, 4 \quad (7.9)$$

$$\xi = \frac{A_{Wt,init.}}{A_{Wt}} \cdot (a \cdot T + b) \quad , \quad (7.10)$$

where k_i^0 is frequency factor and E_i is activation energy and a, b are constants.

Model of the thermal decomposition process based on COD value

The change of COD value should correspond to the change of the components of the sludge, and the weight of each variable roughly represents the components of the sludge. If the COD value is related to the weight, the change of the COD value should be estimated from the model by the weight. A_{COD} , B_{COD} and C_{COD} are plotted against A_{Wt} , B_{Wt} and C_{Wt} , respectively, as shown in Fig.7.16~7.18. These figures show that there may exist a linear relation between the COD value and the weight with respect to each variable. These data are

analyzed by the simple linear regression analysis^[7-14], and the results of this analysis are shown in Table 7.2, Fig.7.16~Fig.7.18. As shown in Table 7.2, the significance of linear regression, the significance of the lack of fit and the 95[%] confidence limit for the parameters of this linear model of the COD against the weight are examined, respectively. From this result, it is shown that these linear models are meaningful and useful. The 95[%] confidence region of the predicted value of the COD is shown by shading in Figs.7.16~7.18.

Finally, the prediction of the change of the COD is made as follows. At first, the weight of each variable is calculated from the model of the thermal decomposition process based on weight, and then the COD values are predicted by these linear regression models.

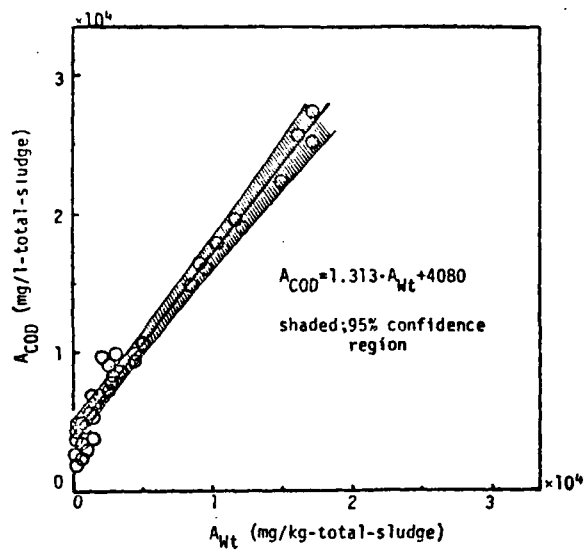


Fig. 7.16 Regression line of A_{COD} against A_{Wt} .

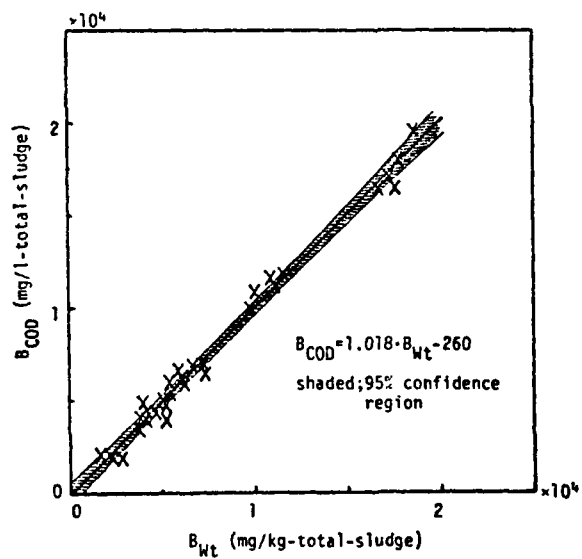


Fig. 7.17 Regression line of B_{COD} against B_{Wt} .

Table 7.2 Linear regression model of COD and weight.

Linear regression model		Each parameter 95% confidence interval	Correlation coeff.
A_{COD} against A_{wt}	$A_{\text{COD}} = 1.313A_{\text{wt}} + 4080$	$1.313 \pm 0.156,$ 4080 ± 660	0.93
B_{COD} against B_{wt}	$B_{\text{COD}} = 1.018B_{\text{wt}} - 260$	$1.018 \pm 0.062,$ -260 ± 610	0.98
C_{COD} against C_{wt}	$C_{\text{COD}} = 0.55C_{\text{wt}} + 1080$	$0.55 \pm 0.17,$ 1080 ± 370	0.73
C_{wt} against C_{COD}	$C_{\text{wt}} = 0.967C_{\text{COD}} + 460$	$0.967 \pm 0.297,$ 460 ± 990	

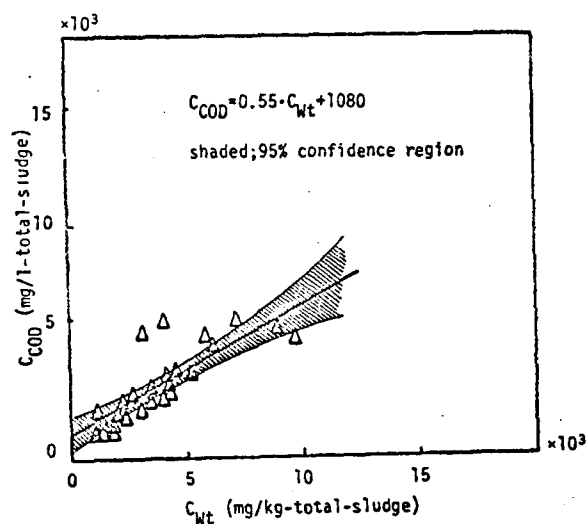


Fig. 7.18 Regression line of C_{COD} against C_{wt} .

7-6. PARAMETER FITTING

The values of parameters in the mathematical model described by Eqs. (7.5)~(7.10) must be determined from experimental data. The mathematical model being considered is described by a set of ordinary differential equations. The parameter fitting of this process is nonlinear one. With respect to nonlinear fitting, much works have been described, and several works employing nonlinear fitting techniques have been reported^{[7-15],[7-16]}. Usually the nonlinear parameter fitting problem is solved using the gradient method and the linearization technique on which are based the local linearization theory. There are various techniques with the gradient method, for example, steepest descent, conjugate gradient^[7-17], Marquardt method^[7-18] etc. Here, the steepest descent method^[7-15] is used. The general procedure of parameter fitting using the steepest descent method is as follows.

A set of ordinary differential equations describing the system is given by

$$\dot{x} = f(x, \theta, t) \quad , \quad x(0) = x_0 \quad , \quad (7.11)$$

where x is the n -dim. column vector of state variables,

f is the n -dim. column vector,

θ is the l -dim. column vector of parameters,

and $x(0)$ means the initial value of x .

The value of the variable x cannot be observed directly, instead observations y_r are made,

$$y_r = g[x(t_r)] + \eta_r \quad r = 1, \dots, R \quad (7.12)$$

where y_r is the m -dim. observation column vector,

g is the m -dim. column vector,

and η_r is the m -dim. vector of random variables affecting the measurement at time t_r .

It is assumed that the form of the function f and g is known together with the statistical properties of the η_r . The problem is to deduce a predicted value $\bar{\theta}$ of the vector of true parameters θ^* from observations of the y_r at time t_r . Usually this problem is solved by finding the values of the θ which minimize a function such as

$$F(\theta) = \sum_{r=1}^R (y_r - g\{x(t_r)\})' \cdot W_r \cdot (y_r - g\{x(t_r)\}) \quad , \quad (7.13)$$

where the weighting matrices W_r are the $m \times m$, symmetric and positive definite and the prime denotes transposing of the vector or matrix. Now the error vector η_r corresponding to different sets of measurements will be assumed to be statistically independent. Hence,

$$E[\eta_r \cdot \eta_s'] = 0 \quad , \quad r \neq s \quad , \quad (7.14)$$

where E represents the expected value. On the other hand, the covariance matrix of the error vector η_r is defined by M_r of

$$E[\eta_r \cdot \eta_r'] = M_r \quad , \quad (7.15)$$

and the error vectors are assumed to have a Gaussian distribution with zero mean. On this assumption the best choice of W_r is led as follows, by the maximum likelihood principle,

$$W_r = M_r^{-1} \quad , \quad (7.16)$$

where -1 denotes the inverse matrix. Then, rewriting the problem,

it is to find the value of θ which minimizes a function such as

$$F(\theta) = \sum_{r=1}^R (y_r - g|x(t_r)|)' \cdot M_r^{-1} \cdot (y_r - g|x(t_r)|) \quad , \quad (7.17)$$

which are subject to Eq.(7.11) and Eq.(7.12).

This problem can be solved by using the steepest descent method as shown below. Considering the first order variation of Eq.(7.11) with respect to nominal value of parameter θ , it is

$$\dot{\lambda} = \frac{\partial f}{\partial x} \cdot \lambda + \frac{\partial f}{\partial \theta} \quad , \quad (7.18)$$

and

$$\lambda(0) = 0 \quad (7.19)$$

where λ is $n \times 1$ matrix of

$$\begin{bmatrix} \frac{\partial x_1}{\partial \theta_1}, \dots, \frac{\partial x_1}{\partial \theta_l} \\ \vdots \\ \frac{\partial x_n}{\partial \theta_1}, \dots, \frac{\partial x_n}{\partial \theta_l} \end{bmatrix} \quad ,$$

$\frac{\partial f}{\partial x}$ is $n \times n$ matrix of

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1}, \dots, \frac{\partial f_1}{\partial x_n} \\ \vdots \\ \frac{\partial f_n}{\partial x_1}, \dots, \frac{\partial f_n}{\partial x_n} \end{bmatrix} \quad .$$

and $\frac{\partial f}{\partial \theta}$ is $n \times l$ matrix of

$$\begin{bmatrix} \frac{\partial f_1}{\partial \theta_1} & \dots & \frac{\partial f_1}{\partial \theta_l} \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial \theta_1} & \dots & \frac{\partial f_n}{\partial \theta_l} \end{bmatrix}$$

And $\partial f / \partial x$ and $\partial f / \partial \theta$ are evaluated at nominal value of parameter θ .

Next, the first order variation of $F(\theta)$ is

$$\delta F = -2 \cdot \sum_{r=1}^R (y_r - g[x(t_r)])' \cdot M_r^{-1} \cdot G_r \cdot \lambda_r \cdot \delta \theta \quad , \quad (7.20)$$

where G_r is the $m \times m$ matrix of

$$\begin{bmatrix} \frac{\partial g_1[x(t_r)]}{\partial x_1} & \dots & \frac{\partial g_1[x(t_r)]}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial g_m[x(t_r)]}{\partial x_1} & \dots & \frac{\partial g_m[x(t_r)]}{\partial x_n} \end{bmatrix} \quad ,$$

λ_r is the matrix λ evaluated at $t=t_r$ and these matrices or vectors are evaluated at the nominal value of parameter θ . The necessary condition of this minimization problem is $\delta F=0$. Generally at nominal value of parameter θ , this condition may not be satisfied. Then θ is corrected in the direction of the maximum gradient of F with respect to θ . From the condition of local linearization,

$$\delta \theta' \cdot Z \cdot \delta \theta = S^2 \quad , \quad (7.21)$$

where the weighting matrix Z is $l \times l$ symmetric positive definite,

and S^2 is the measure suitably chosen. By the simple calculation using Eq.(7.20) and Eq.(7.21), the corrected stepsize $\delta\theta$ of the parameter θ is given as,

$$\delta\theta = \frac{1}{\mu} \cdot \left[\sum_{r=1}^R Z^{-1} \cdot \lambda_r' \cdot G_r' \cdot M_r^{-1} \cdot (y_r - g(x(t_r))) \right] \quad (7.22)$$

where μ satisfies the relation of

$$\begin{aligned} \mu^2 \cdot S^2 = & \left[\sum_{r=1}^R (y_r - g(x(t_r))) \cdot M_r^{-1} \cdot G_r \cdot \lambda_r \right] \cdot Z^{-1} \times \\ & \times \left[\sum_{r=1}^R \lambda_r' \cdot G_r' \cdot M_r^{-1} \cdot (y_r - g(x(t_r))) \right] \end{aligned} \quad (7.23)$$

Then the corrected θ_{new} is

$$\theta_{\text{new}} = \theta + \delta\theta \quad (7.24)$$

This procedure must be continued till the value of δF becomes as small as approximately zero.

On the other hand, the confidence intervals for the fitted parameter $\bar{\theta}$ can be calculated by using unit vector b [7-15] and is based on a confidence interval $\gamma(b)$ with the projection of $\bar{\theta}$ upon any unit vector b . When H is defined as follows

$$H = \sum_{r=1}^R \lambda_r' \cdot G_r' \cdot M_r^{-1} \cdot G_r \cdot \lambda_r \quad (7.25)$$

and $\Delta\theta$ is defined by $\Delta\theta = \theta^* - \bar{\theta}$, then the linear function of $\Delta\theta$, $b' \Delta\theta$ will take Gaussian distribution with variance of

$$\sigma_b^2 = b' H^{-1} \cdot b \quad (7.26)$$

where b is a unit L -vector.

The confidence interval $\gamma(b)$ associated with $b'\bar{\theta}$ is then

$$\gamma(b) = K \cdot \sigma_b \quad (7.27)$$

where K depends on the chosen confidence level. For example at 95 per cent level $K=1.96$. Hence if we assume that

$$b'\bar{\theta} - 1.96 \cdot \sigma_b \leq b'\theta^* \leq b'\bar{\theta} + 1.96 \cdot \sigma_b \quad (7.28)$$

then, we shall be correct on 95 per cent of the occasions. The method described above can therefore be applied to our problem.

For simplicity, at first the parameters of k_1, k_2, k_3, k_4 in Eqs.(7.5) ~ (7.7) are fitted from the experimental data with the condition of constant temperature. The experiments of Runs (7-1)~(7-6) cited in Table 7.1 are performed under the condition of constant temperature, and the values of k_1, k_2, k_3, k_4 are fitted from the experimental data of Run (7-1) ~ Run (7-6). The fitted parameters k_1 in each run are shown in Table 7.3. From this result the constants a, b in Eq.(7.13) are fitted by using the plot of $A_{Wt,sat.}/A_{Wt,init.}$ against the temperature T . This plot is shown in Fig.7.19. From this figure, ξ is given as

$$\xi = \frac{A_{Wt,init.}}{A_{Wt}} \cdot (-0.00457 \cdot T + 2.323) \quad (7.29)$$

where T has a unit of $^{\circ}\text{K}$.

The calculated values using the values of these fitted parameters obtained for each run, are shown by the solid curves in Figs.7.4_a~7.9_a. Moreover, by using the result of the Arrhenius plot of these predicted parameters k_1 for the initial assumed parameter values, the parameters in Eq.(7.9) are fitted from the experi-

mental data of Run (7-7) by the previously described technique.

For this case the procedure of parameter fitting should be modified, slightly. The nomenclatures in Eqs.(7.5)~(7.10) correspond to those in the procedure described above and C_{Wt} in Eq.(7.7), substituted in Eq.(7.5) and Eq.(7.6), then,

$$x' = (A_{Wt}, B_{Wt}) \quad (7.30)$$

$$\theta' = (k_1^0, k_2^0, k_3^0, k_4^0, E_1, E_2, E_3, E_4) \quad (7.31)$$

$$f = \begin{bmatrix} -(k_1^0 \cdot e^{\frac{-E_1}{R \cdot T}} + k_2^0 \cdot e^{\frac{-E_2}{R \cdot T}}), & 0 \\ k_1^0 \cdot e^{\frac{-E_1}{R \cdot T}} - k_4^0 \cdot e^{\frac{-E_4}{R \cdot T}}, & -(k_3^0 \cdot e^{\frac{-E_3}{R \cdot T}} + k_4^0 \cdot e^{\frac{-E_4}{R \cdot T}}) \end{bmatrix} \times \begin{bmatrix} A_{Wt}(1-\xi) \\ B_{Wt} \end{bmatrix} \quad (7.32)$$

$$x'(0) = (A_{Wt,init.}, B_{Wt,init.}) \quad (7.33)$$

Considering the procedure of the measurement of weight, then

$$y_r = \begin{bmatrix} (A_{Wt} + B_{Wt}) \\ (B_{Wt}) \end{bmatrix} \text{observed value at } t_r \quad (7.34)$$

For the simplicity M_r and Z are taken as,

$$M = I \cdot \sigma^2 \quad r = 1, \dots, R \quad (7.35)$$

$$Z = I \quad (7.36)$$

where I is unit matrix and σ^2 is taken as $6 \times 10^3 [\text{mg/kg-total-sludge}]^2$ from the other experiment.

By using these relations, the parameters in Eq.(7.31) are fitted from the experimental data of Run (7-7) as shown in Table 7.4 and they are compared with each other by the Arrhenius plot as shown in Fig.7.20, where various signs show the rate constants given by Run (7-1) ~ Run (7-6) and the straight lines show one given by Run (7-7). It is also seen that the value of k_2 given by Run (7-1) ~ Run (7-6) is almost the same as that given by Run (7-7), but that the other parameters do not agree in both cases. However, investigating the confidence regions of fitted parameters, the degree of this difference may be estimated. For example, with respect to Run (7-4) 95 per cent parameter confidence regions are given in Table 7.5. If b is taken so that $b_i=1$; $b_j=0$, $j \neq i$ for k_i , the confidence interval for an element k_i is found as in Table 7.5. The confidence interval by the projection of $\bar{\theta}$ on the eigen vector of H^{-1} has a further advantage, but it can be generally recognized that the fitted parameters have wide confidence regions. Averaging the values of the fitted parameters given from Run (7-1) ~ Run (7-7), the mathematical model of the thermal decomposition process based on weight becomes

$$\frac{dA_{Wt}}{dt} = -(0.37 \cdot e^{-\frac{249}{T}} + 0.319 \cdot e^{-\frac{500}{T}}) \cdot (1-\xi) \cdot A_{Wt} \quad , \quad (7.37)$$

$$\frac{dB_{Wt}}{dt} = 0.37 \cdot e^{-\frac{249}{T}} \cdot (1-\xi) \cdot A_{Wt} - 1800 \cdot e^{-\frac{4600}{T}} \cdot B_{Wt} + 0.55 \cdot e^{-\frac{1260}{T}} \cdot C_{Wt} \quad , \quad (7.38)$$

$$C_{Wt} = (A_{Wt} + B_{Wt})_{\text{init.}} - A_{Wt} - B_{Wt} \quad , \quad (7.39)$$

Table 7.3 Estimated parameter value.

Run No.	k_1 (1/min)	k_2 (1/min)	k_3 (1/min)	k_4 (1/min)
7-1	0.5	0.095	0.00395	0.00736
7-2	0.5	0.095	0.0146	0.0306
7-3	0.5	0.095	0.00907	0.0150
7-4	0.5	0.095	0.183	0.0249
7-5	0.5	0.095	0.0123	0.0618
7-6	0.5	0.095	0.00645	0.0153

$$\zeta = (-0.00457T + 2.3230) A_{Wt, \text{init.}} / A_{Wt}$$

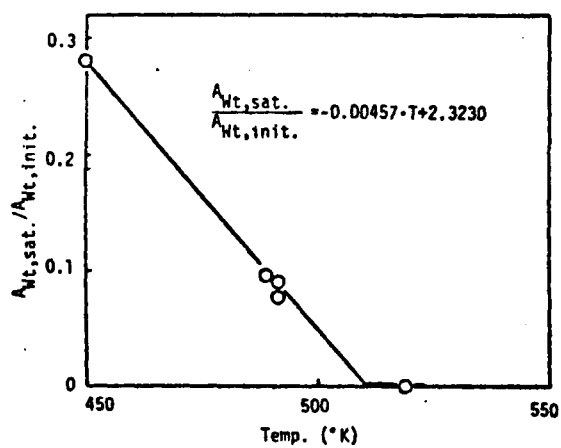


Fig. 7.19 $A_{Wt, \text{sat.}} / A_{Wt, \text{init.}}$ vs. T.

Table 7.4 Estimate parameter
value from Run 7-7.

$$\begin{aligned} k_1 &= 0.245 \cdot \exp(-497/T) \\ k_2 &= 0.319 \cdot \exp(-500/T) \\ k_3 &= 3100 \cdot \exp(-5800/T) \\ k_4 &= 0.90 \cdot \exp(-1500/T) \end{aligned}$$

Table 7.5 An example of parameter confidence regions,
at a level 0.95, Run7-4.

$$bk - 1.96 \cdot \sqrt{bHb} \leq bk^* \leq bk + 1.96 \cdot \sqrt{bHb}$$

where H is,

$$H = \begin{bmatrix} 0.88 \times 10^{-4}, & -0.12 \times 10^{-6}, & -0.29 \times 10^{-4}, & -0.17 \times 10^{-6} \\ -0.12 \times 10^{-6}, & 0.83 \times 10^{-9}, & 0.50 \times 10^{-7}, & -0.13 \times 10^{-8} \\ -0.29 \times 10^{-4}, & 0.50 \times 10^{-7}, & 0.10 \times 10^{-4}, & 0.74 \times 10^{-7} \\ -0.17 \times 10^{-6}, & -0.13 \times 10^{-8}, & 0.74 \times 10^{-7}, & 0.20 \times 10^{-8} \end{bmatrix}$$

In the case of $b_i = 1, b_j = 0, i \neq j$,

$$\begin{aligned} k_1 - 1.4 &\leq k_1^* \leq k_1 + 1.4 \\ k_2 - 0.0043 &\leq k_2^* \leq k_2 + 0.0043 \\ k_3 - 0.48 &\leq k_3^* \leq k_3 + 0.48 \\ k_4 - 0.0055 &\leq k_4^* \leq k_4 + 0.0055 \end{aligned}$$

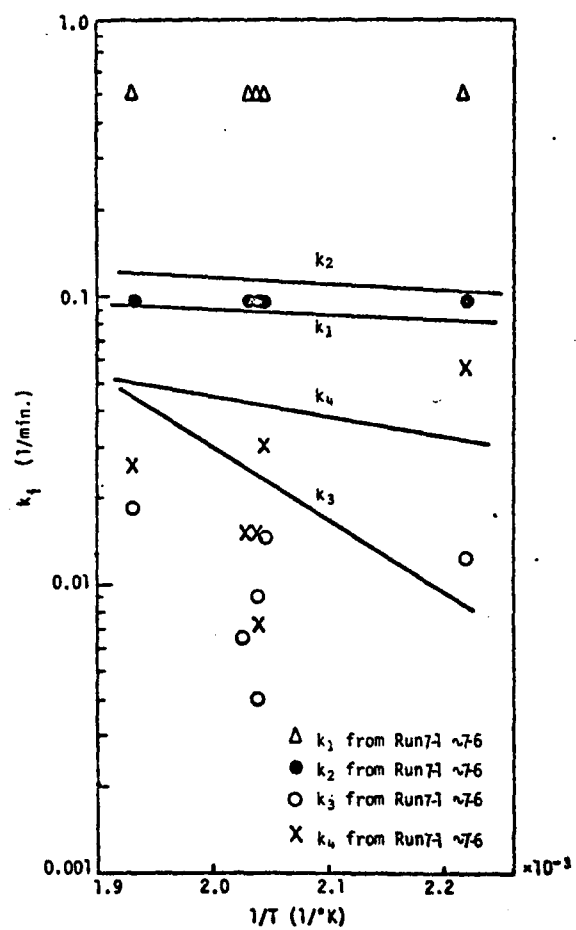


Fig. 7.20 Arrhenius plot of the fitted parameters.

where

$$\xi = \frac{A_{Wt,init.}}{A_{Wt}} \cdot (-0.00457 \cdot T + 2.323) \quad .$$

Next, the calculated COD values for each run are shown by Fig.7.4, ~Fig.7.10_b by using the fitted parameters shown in Table 7.3 and Table 7.4, respectively and by using the regression lines of the COD against the weight. In these figures the confidence regions at 95 per cent level of the predicted COD values are shown by shading. The predicted COD values do not fit the experimental data as well as the weight.

The calculated COD and W_t values for each run explains the experimental data by using the parameter values shown in Table 7.4.

7-7. DISCUSSION OF THE MODEL

It has been assumed that the initial soluble matter is of the same class as the soluble matter. Whether this assumption is reasonable or not has been considered from the experiments in which only the initial soluble matter reacts. The data for this experiment are shown in Fig.7.11. The dotted curve in this figure represents the calculated value by using the model. It is seen from this consideration that the above assumption is not so unreasonable. As described previously, the plot of $\frac{1}{T}$ vs. the ratio of C_{Wt} to B_{Wt} at a steady state becomes the straight line as shown in Fig.7.15. From this straight line, $E_3/R - E_4/R = 3900$ and $k_3^o/k_4^o = 1.4 \times 10^3$. On the other hand from the fitted parameter values, $E_3/R - E_4/R = 3340$ and $k_3^o/k_4^o = 3.2 \times 10^3$. Therefore it may be concluded that the estimation of the parameters of k_3^o, k_4^o, E_3 and E_4 are adequate

It may be doubtful whether this model can be used beyond the range of our experimental conditions. However, it is apparent that behaviour similar to this model can generally be seen in the experiments of other workers.

7-8. CONCLUDING REMARKS

It is confirmed by using artificially cultured activated sludge that the reaction of thermal decomposition has an important role in the treatment of sludge. A mathematical model of this reaction is proposed^[7-4] based on the experimental data, and the values of the parameters of this model are estimated by using the steepest descent method.

NOMENCLATURE

A ; solid matter

B ; soluble nonevaporative matter

C ; soluble evaporative matter

COD; Chemical Oxygen Demand [mg/l-total-sludge]

f ; function of state variable

g ; observing function

k_i ; reaction rate constant

M_i ; covariance matrix of random error

T ; temperature [$^{\circ}$ K]

t ; time [min]

X ; matrix constructed by state vector

x ; vector of state variables

y_i ; observe value vector

W_i ; weighting matrix

W_t ; weight [mg/kg-total-sludge]

θ ; parameter vector

$\Delta\theta$; small deviation of parameter

λ ; sensitivity coefficient of x with respect to

σ_b^2 ; variance

η ; error vector

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CHAPTER 8

SYSTEM IDENTIFICATION OF WET-AIR OXIDATION PROCESS-II OXIDATION

8-1. INTRODUCTORY REMARKS

As already shown in Chapter 7, the thermal decomposition reaction exists in the wet-air oxidation process, and a mathematical model of the same process was proposed. It is the purpose of this chapter to identify the mathematical model for the oxidation process. The oxidation process means the reaction in which the sludge is oxidized by oxygen under the conditions of a temperature of 170-250°C and a pressure of 60-130 kg/cm²-gauge. This process is the so called, Zimmermann Process [8-1],[8-3]. To identify this model, the model of the thermal decomposition process is partially used, because it's a known fact that the solid matter is decomposed into soluble matter by the oxidation as well as the thermal decomposition process. The mathematical model developed in this chapter [8-4] is expressed and identified by the state variables of COD and weight of solid matter, soluble non-evaporative and evaporative matter, as well as by a thermal decomposition model [8-5]. Also, the parameters of this mathematical model are estimated by nonlinear estimation techniques.

8-2. STATE VARIABLES

The results of the previous chapter again stated are briefly here:

- (i) The state variables describing the mathematical model of thermal decomposition are the COD and the weight of solid matter, soluble non-evaporative and evaporative.
- (ii) The model of the thermal decomposition process with respect to the weight is shown in Fig.8.1. All reaction paths of this model are first order.
- (iii) The change of the COD value in the thermal decomposition process is estimated from the regression line of COD against the weight.

Now, consider that the mathematical model of the oxidation process depends on these variables of COD and weight of solid matter (A), soluble nonevaporative matter (B) and soluble evaporative matter (C) in the sludge as well as the thermal decomposition model because these variables grossly represent the contents of the sludge. These variables are defined from experimental measurements as shown in the previous chapter, but the weight of the soluble evaporative matter (C_{Wt}) cannot be calculate from the mass balance of the weight of the solid matter (A_{Wt}), the weight of the soluble nonevaporative matter (B_{Wt}) and the weight of the soluble evaporative matter (C_{Wt}), because matter other than A, B, C is produced by oxidation. These products are mainly CO_2 and water, but there is also some CO and other gases. Hereafter the matter produced by oxidation, other than A, B, C, is denoted by P.

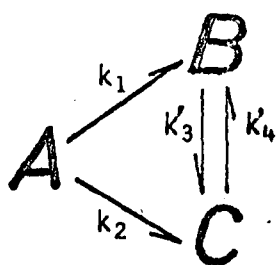


Fig. 8.1 Thermal decomposition model.

Then, if P_{Wt} can be directly measured, C_{Wt} can be calculated, but the weight of the water produced by oxidation cannot be measured directly though the weight of produced gas can be analyzed quantitatively. The weight of the produced water will be calculated from the weight of produced gas under a certain assumption. The preciseness of the quantitative analysis of gas is frequently poor because of the limitation of the experimental technique. Furthermore, the number of the gas samplings in the batch type experiment is limited because the gas sampling causes a wide change of the experimental conditions. Then, C_{Wt} is calculated another way as shown below. It is assumed that the regression line of C_{Wt} against C_{COD} in the oxidation process is the same line as that in the thermal decomposition process. On the other hand, COD value of the soluble evaporative matter (C_{COD}) can be calculated by subtracting B_{COD} from the COD value of the soluble matter considering the COD value of P to be zero. Then, C_{Wt} is calculated by using the regression line of C_{Wt} against C_{COD} .

8-3. RELATIONSHIP BETWEEN THERMAL DECOMPOSITION AND OXIDATION

The model of the thermal decomposition process is partially useful for the model identification of the oxidation process for the reasons mentioned next. Using artificial cultured activated sludge, both experiments of oxidation and thermal decomposition are held under the same conditions except for the initially contained in the reactor. That is to say, the difference in both experiments depends on whether the gas initially contained in the free space of the reactor is oxygen or nitrogen. The reactor is a magnetically stirred type autoclave the volume of which is 500cc. The results of these experiments are shown in Fig.8.2 and Fig.8.3. As shown in these figures, the change of the weight and the COD of the soluble evaporative matter are quite different in both cases of oxidation and thermal decomposition. On the other hand the weight and the COD value of the solid matter change quite similarly in the oxidation process as well as in the thermal decomposition process. Then, the change of the solid matter in the oxidation process depends on the other experimental conditions, except for oxygen. In the model of the oxidation process with respect to the weight, the reactions of A_{wt} are absolutely the same as in the model of the thermal decomposition process. So, the model of the thermal decomposition process is partially used for the oxidation model. After all, it is said that in the oxidation process the solid matter is once decomposed into soluble matter by thermal decomposition, and then it is oxidized by the oxidation process.

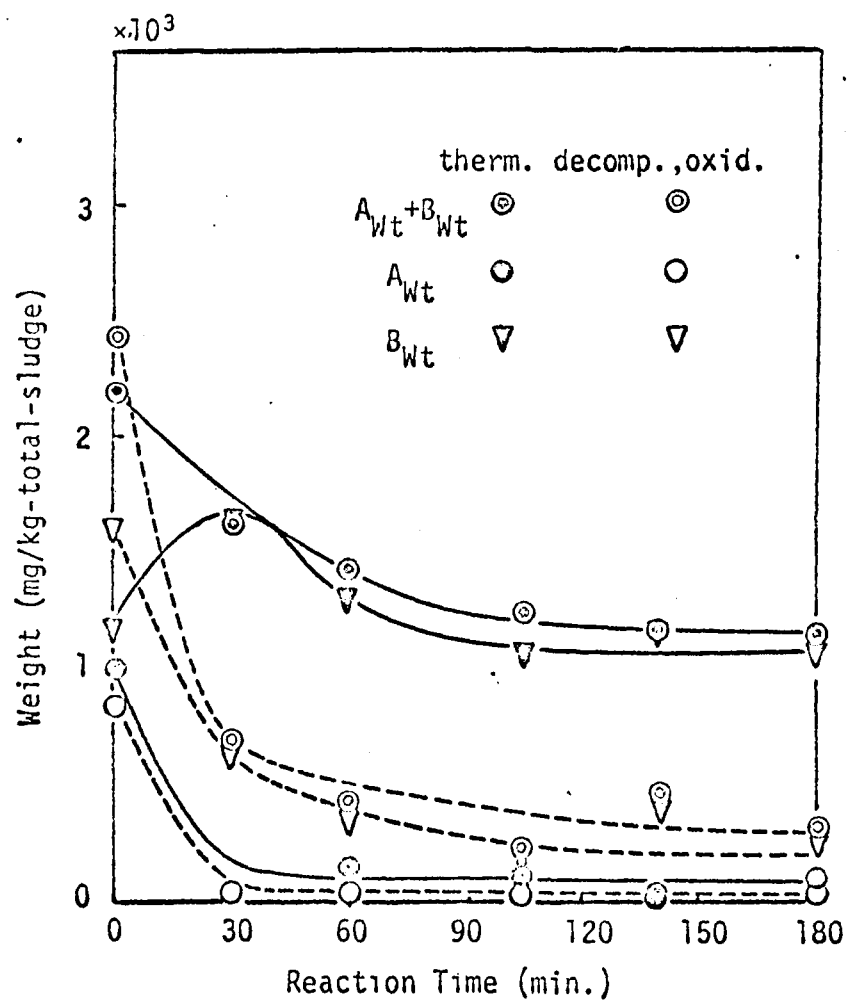


Fig. 8.2 Comparison of oxidation and thermal decomposition with respect to weight.

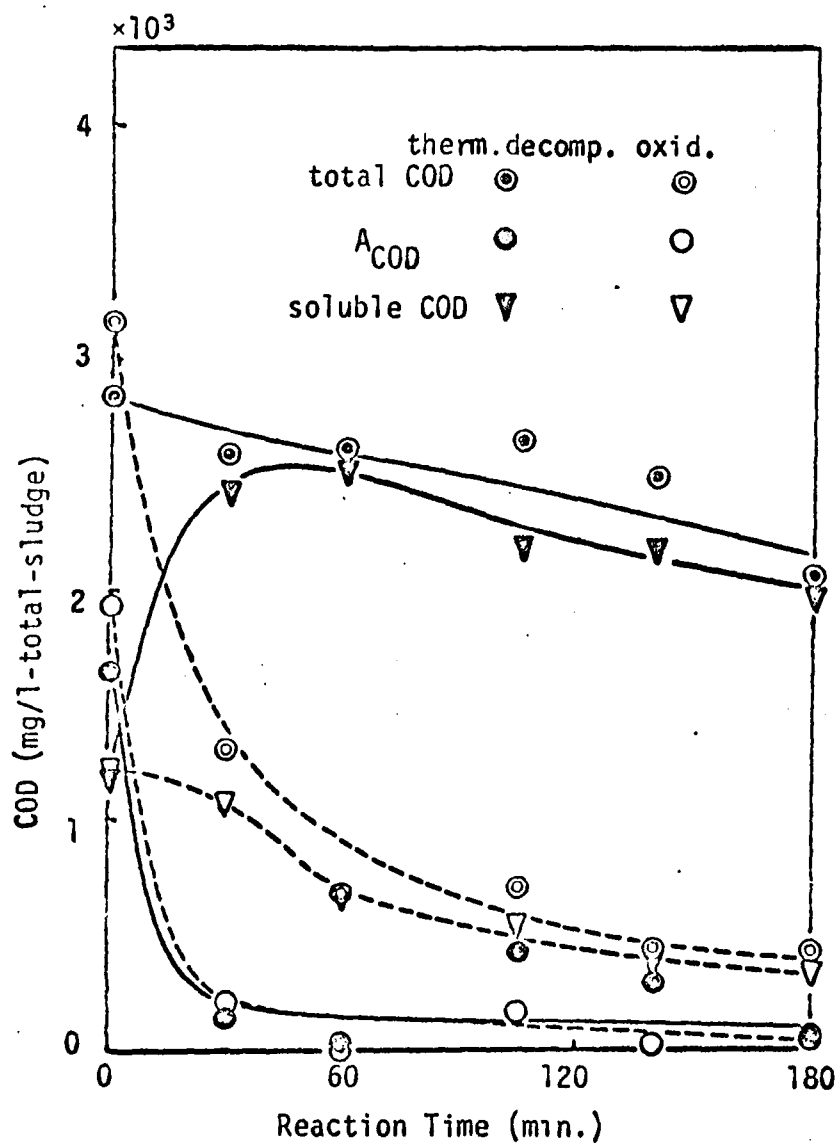


Fig. 8.3 Comparison of oxidation and thermal decomposition with respect to COD.

8-4. EXPERIMENT

To identify the mathematical model of the oxidation process, several experiments are performed.

Sample; The same activated sludge as used for the experiments of the thermal decomposition process is used for this sample. That is to say, the artificially cultured, activated sludge is preserved at a very low temperature of about -60°C and used for the sample.

Equipment; The equipment used for the experiment of the oxidation process is shown in Fig.8.4. An autoclave is used and the reactor has a volume of 500cc, and it's inside is mixed by a magnetic up and down type stirrer. This mixing is considered to be complete. The pressure of the reaction is measured by a pressure gage of the Bourdon type, and the temperature is measured by an A-C thermocouple. Two gas and liquid sampling valve are attached to the reactor. One is used for introducing nitrogen and the other is used for introducing oxygen and gas sampling. The electric furnace is set outside the autoclave.

A substitutional of gas sampler is filled with a saturated solution of salt because CO_2 is not absorbed. The sampling gas is analyzed by gas-chromatography.

Procedure; The frozen sample is warmed and dissolved indirectly by warm water. The reactor is filled with this sample of 250cc, and the inside of the reactor is highly pressurized by nitrogen. The free space of the reactor is filled only with nitrogen by substitution. One of the reasons for the reactor being filled not with oxygen but nitrogen is because the heat capacity of the reactor is large, and so the temperature of the reactor

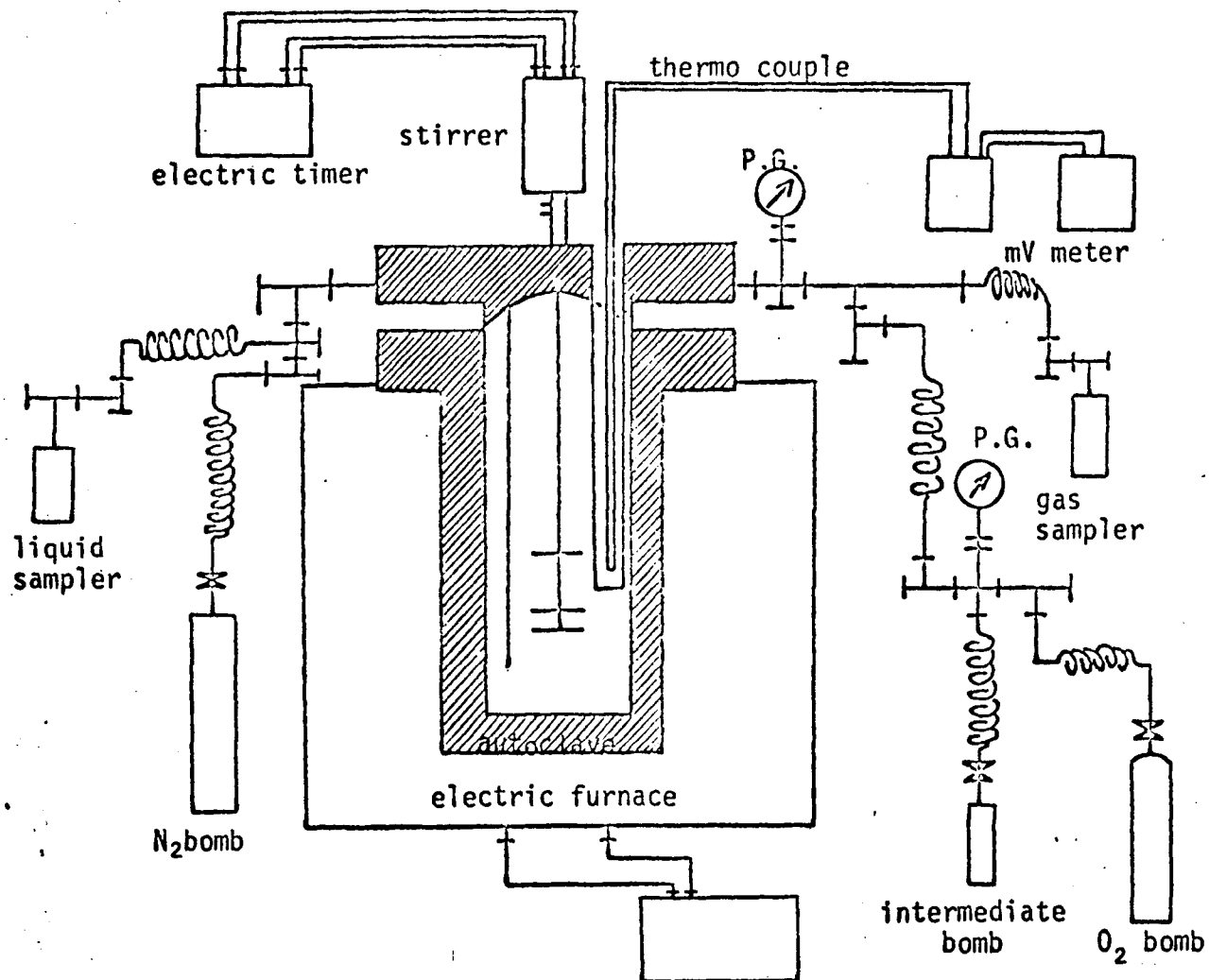


Fig. 8.4 Sketch diagram of the equipment.

cannot be made to increase too fast. That is to say, to perform the experiment under the condition of constant temperature, it is better that oxygen is not contained initially in the reactor. On the other hand, the change of the solid matter in the oxidation process is absolutely the same as in the thermal decomposition process. The model of the change of soluble matter B, C is identified. Another reason for the reactor being initially filled with nitrogen is that it is better to start the oxidation process when soluble matter occupies a large part of the sample.

Next, the temperature of the reactor is made to increase by using an electric furnace. At a suitable temperature which is a steady state, oxygen is poured into the reactor. The volume of oxygen in the reactor has been set so as to be much larger than the theoretical volume calculated by the COD value of the sludge. Then, liquid and gas sampling are carried out at the desired any time. From this sample liquid, the weight and the COD value of each variable are measured. On the other hand this sampled gas is analyzed by gas chromatography. As mentioned above, the result of the analysis of the gas is not used for the quantitative analysis of the experimental data but for qualitative understanding. So, gas sampling is carried out at the beginning and end of the experiment.

Measurement of state variables; The weight and the COD value of solid matter (A) and soluble non-evaporative matter (B) are measured directly or indirectly as shown in the previous chapter. The weight of the soluble evaporative matter (C_{wt}) is estimated by the regression line C_{wt} against C_{COD} .

It is assumed that this estimated value of C_{wt} is the observed value. The reason that this assumption is necessary will be given later.

Experimental conditions; The three elements of initial concentration, temperature and pressure are considered as the experimental conditions. These conditions are shown in Table 8.1 and Fig.8.5. The conditions shown in Table 8.1 are those when oxygen is poured into the reactor. Initially it was intended that the temperature of the reactor was to be kept constant throughout the reaction, but it could not be done because of the difficulty of the operation technique. The value of the fixed suspended matter is also shown in Table 8.1.

Result; The results of the experiments are shown in Fig.8.6~Fig.8.11. Each run number in these figures corresponds to one shown in Table 8.1. The various signs in these figures show the experimental data, and the solid curves show the value calculated by the model to be described later. In Fig.8.6a, the weight of soluble non-evaporative matter (B_{Wt}) decreases at time passes. The higher the temperature of the reactor is, the more quickly B_{Wt} decreases. The reaction consuming B apparently depends on the temperature. On the other hand, the weight of the soluble evaporative matter (C_{Wt}) increases gradually and saturates when the temperature is low as shown in some of the figures. When the temperature is high, C_{Wt} increases once and then decreases as shown in another figure. The reaction producing or consuming C is not one, and the reaction paths of C_{Wt} are affected by the temperature.

Secondly, A_{Wt} does not change much because the initial concentration is small. It is natural to say that the change of A_{Wt} is followed by the model of the thermal decomposition process, in spite of small change A_{Wt} . Finally, the change of the COD is similar to the change of the weight with respect to the shape. The larger deviation of the COD value may be mainly due to experimental errors of the COD method.

Table 8.1 Conditions of the experiments.

Run No.	B _{Wt,init.} (mg/kg)	B _{COD,init.} (mg/l)	Fixed susp. matter (mg/kg)	Temp. (°K)	Press. (kg/cm ²)
8-1	5790	5900	1270	485	70
8-2	4390	4840	1310	520	71~72
8-3	5990	6480	1250	477	67~70
8-4	9620	11700	5780	496	72~75
8-5	17800	19400	4090	498	70~72
8-6	5560	6660	1480	506	110~130

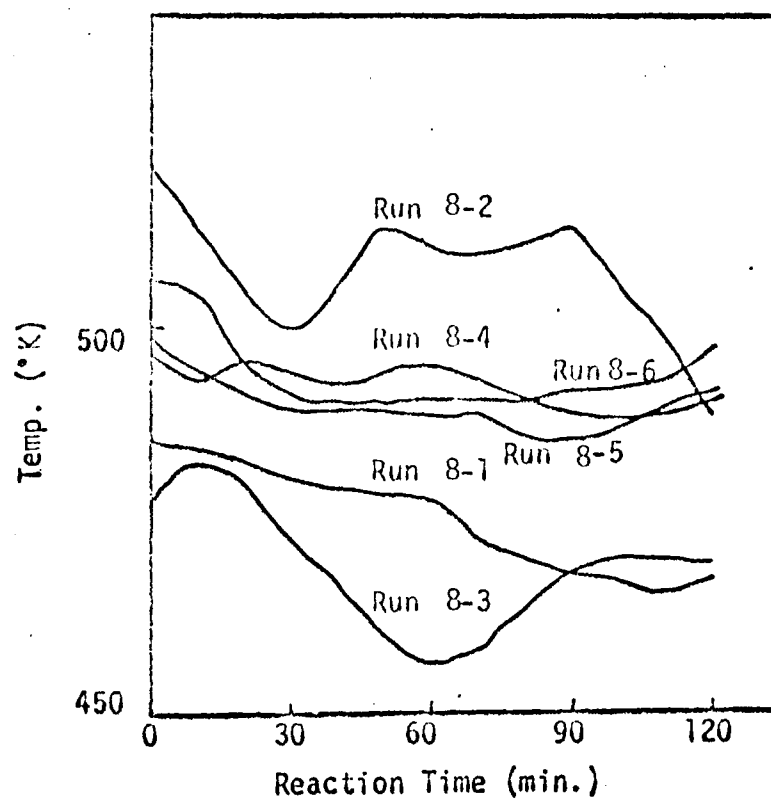


Fig. 8.5 Temperature in the reaction.

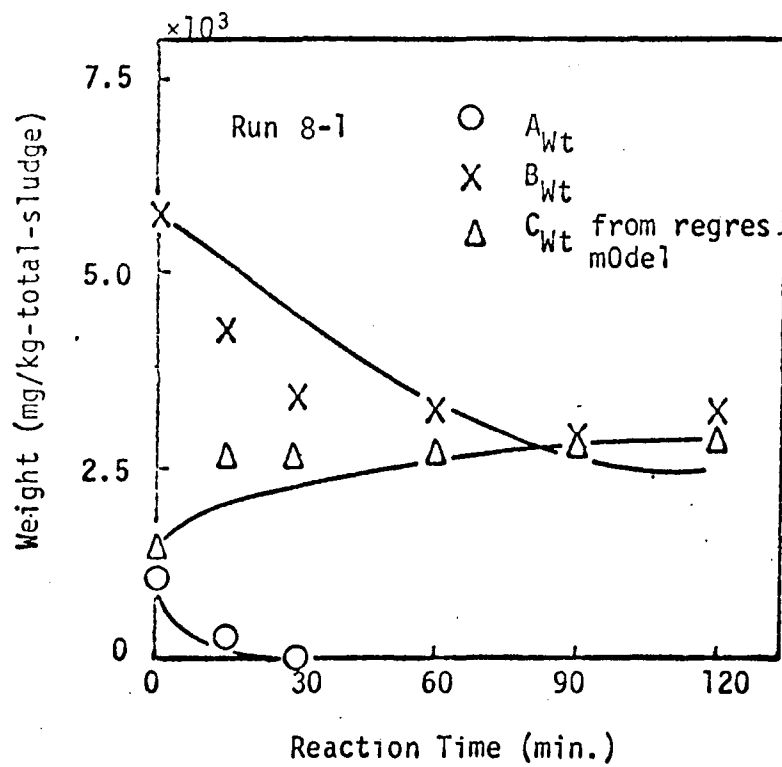


Fig. 8.6_a Change of the weight.

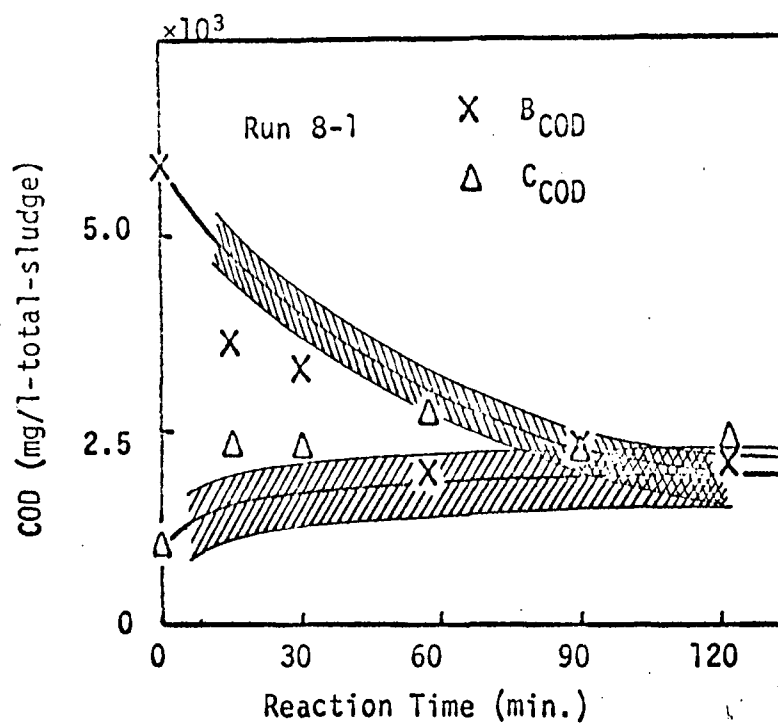


Fig. 8.6_b Change of the COD.

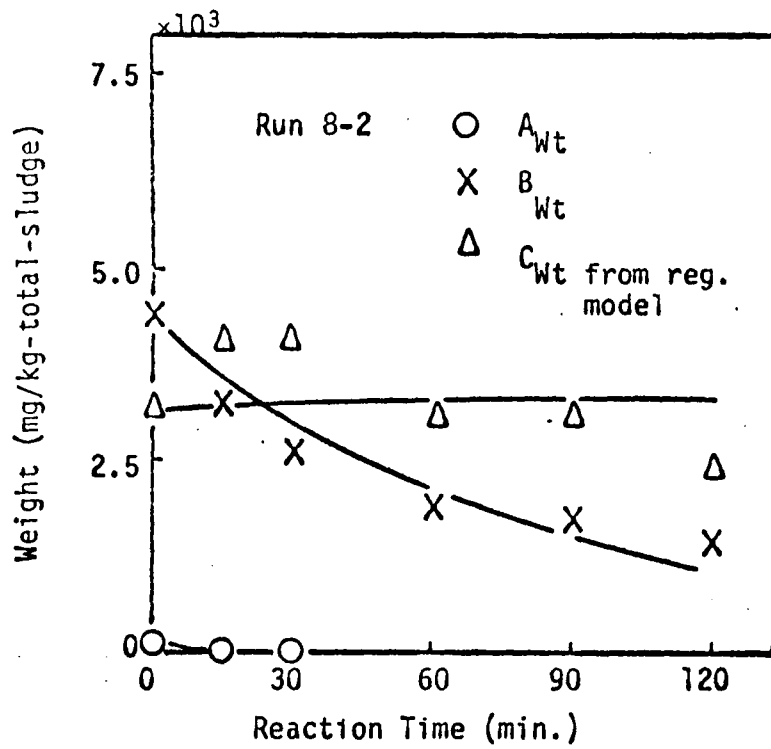


Fig. 8.7_a Change of the weight.

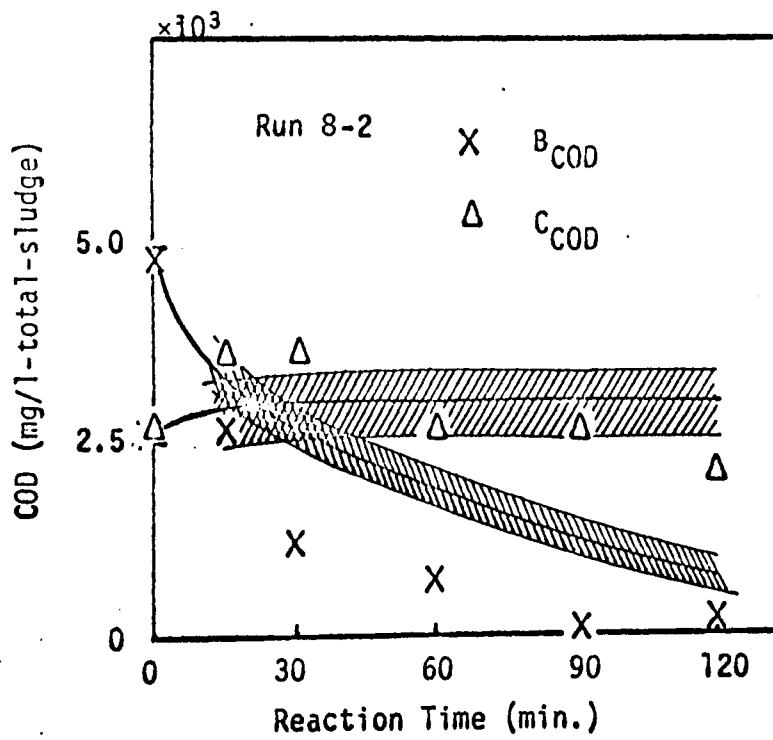


Fig. 8.7_b Change of the COD.

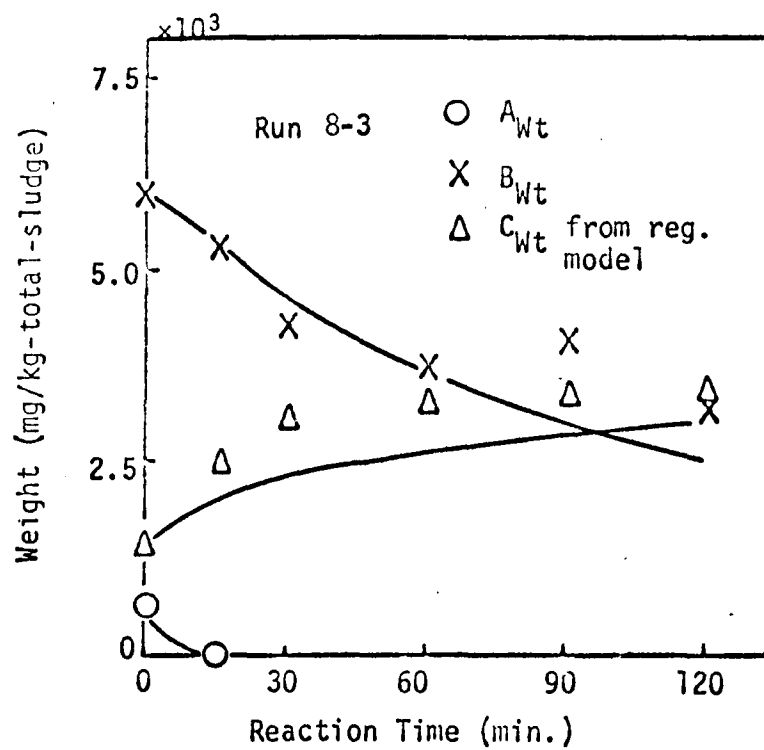


Fig. 8.8_a Change of the weight.

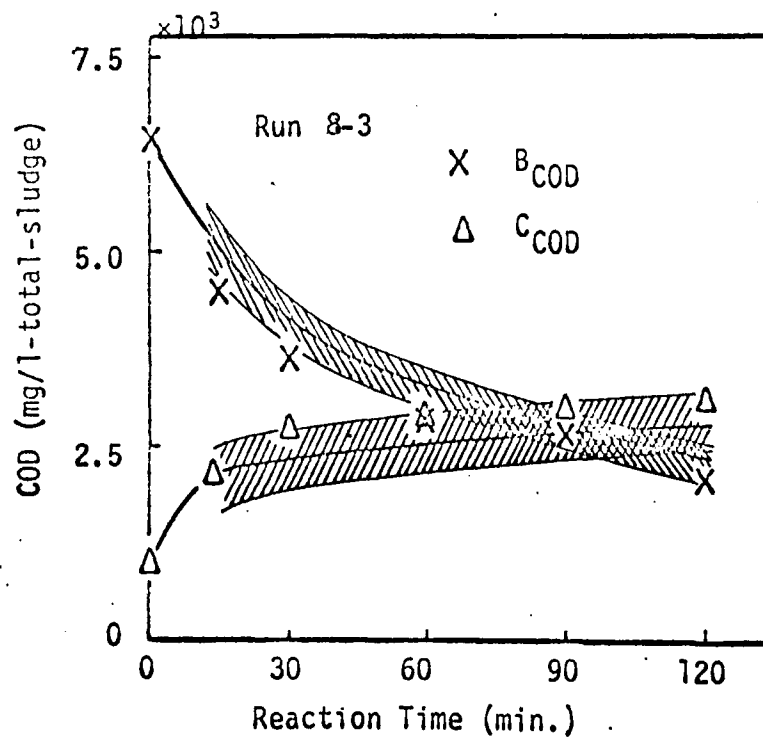


Fig. 8.8_b Change of the COD.

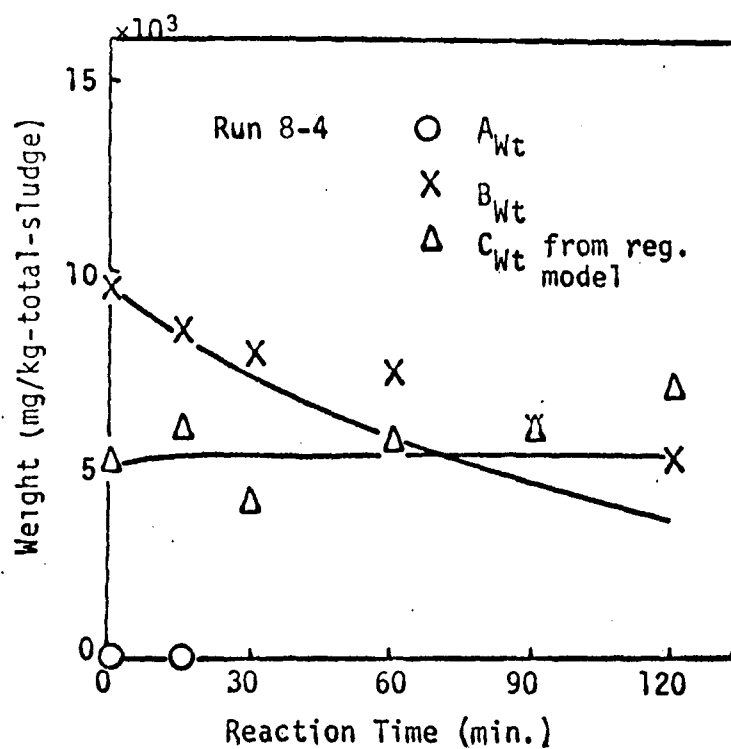


Fig. 8.9_a Change of the weight.

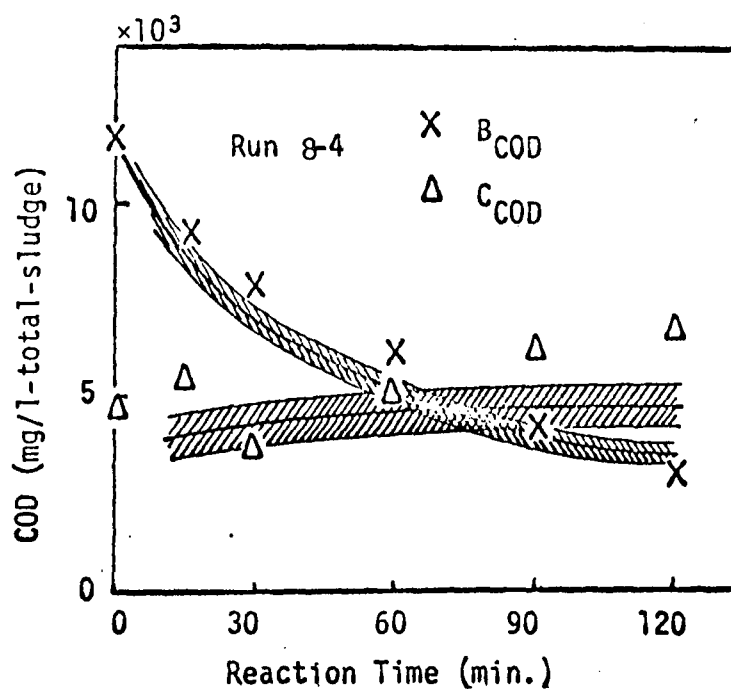


Fig. 8.9_b Change of the COD.

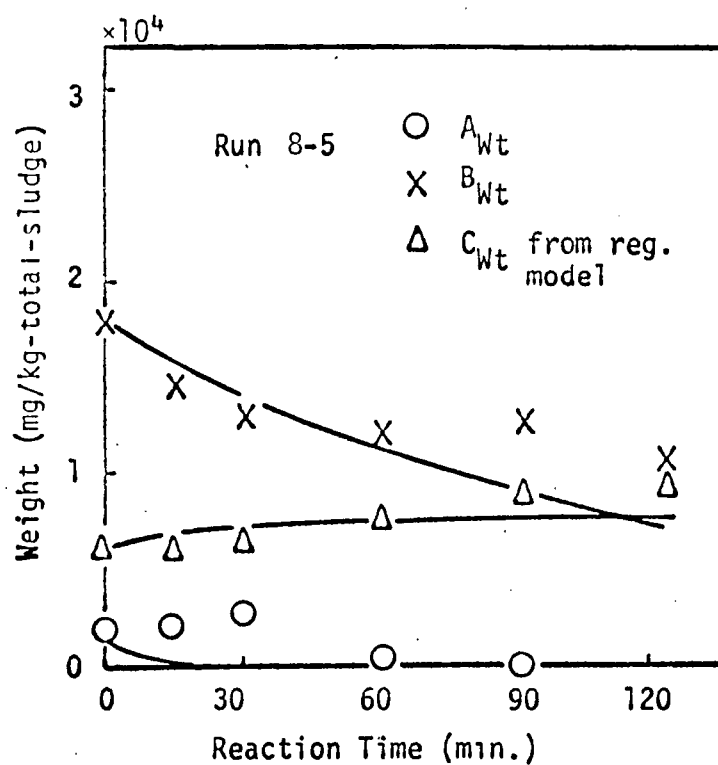


Fig. 8.10_a Change of the weight.

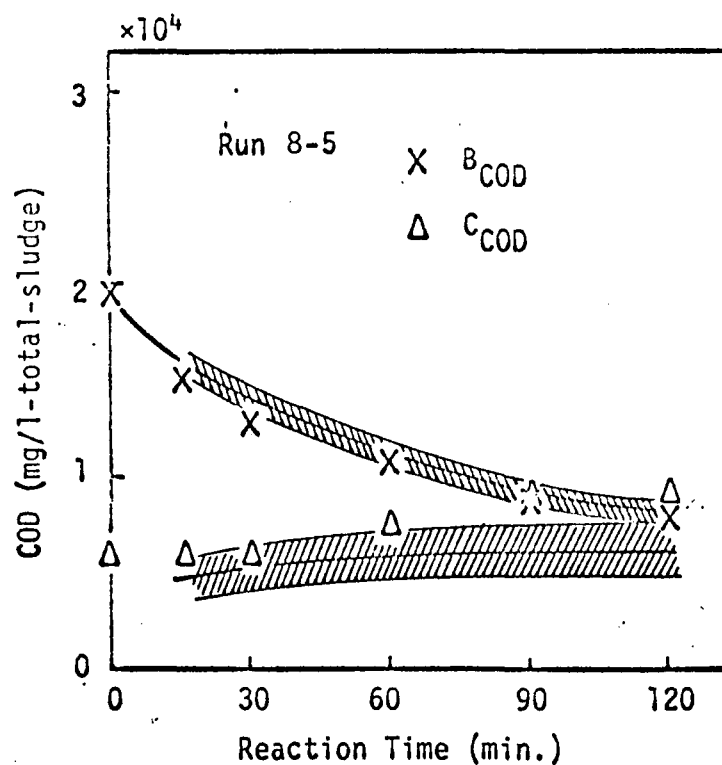


Fig. 8.10_b Change of the COD.

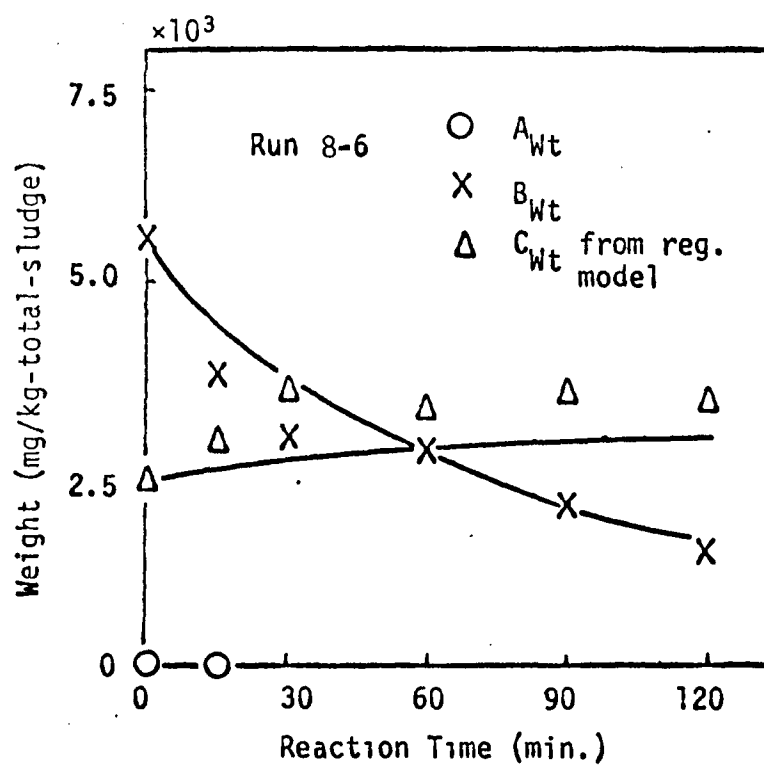


Fig. 8.11_a Change of the weight.

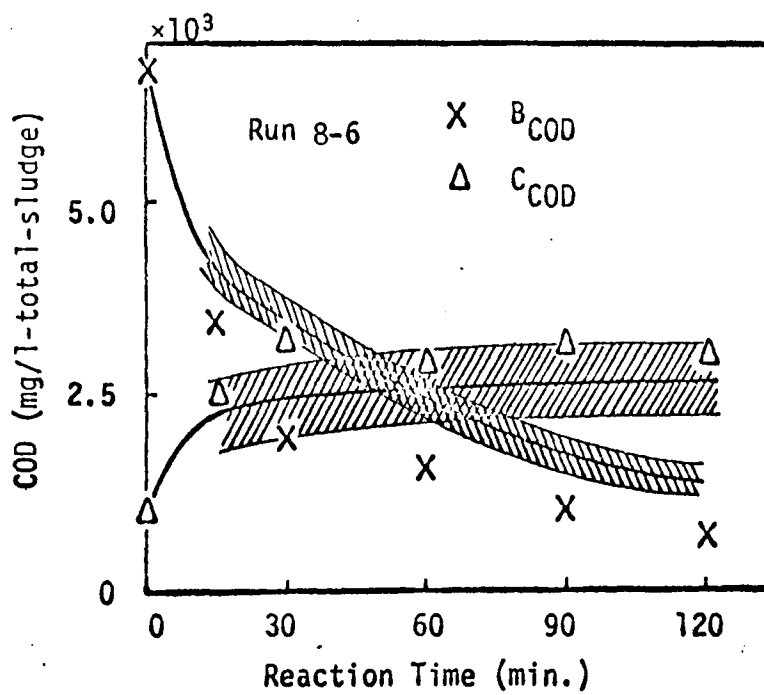


Fig. 8.11_b Change of the COD.

From the similarity in the shape of the change between the weight and the COD, it will be said that the COD values of each variable is estimated by the linear regression relationships of the COD and the weight in the oxidation as well as in the thermal decomposition process.

8-5. MATHEMATICAL MODEL

We will identify the mathematical model of the oxidation process from the results of the experiments. First, a model with respect to the weight is constructed by A_{Wt} , B_{Wt} , C_{Wt} and P_{Wt} . Then the COD values of each variables are estimated by using the linear regression model of the COD against the weight because the change of the COD value is explained as the change of the components of the sludge, and the weight of each variable roughly represents the components of the sludge. It is assumed that the linear regression models of the COD against the weight in the oxidation process are the same as in the thermal decomposition process. From Chapter 7, these regression models are shown in Table 8.2.

The linear regression model of C_{Wt} against C_{COD} is also shown in Table 8.2. This regression line is used for the prediction of C_{Wt} in the oxidation process.

Here, only the model of the oxidation process with respect to the weight is identified. The volume of oxygen in the reactor is much greater than the theoretical volume calculated by the COD value of the sludge. Then, it is assumed that oxygen is not the controlling stage of the oxidation process in this experiment. As previously described, it will be natural to assume that the reaction paths of A_{Wt} in the model of the oxidation process are absolutely the same as in the model of the thermal decomposition process. Namely, the reaction paths of A to B and C exist as shown in Fig.8.1, and the rate constants k_1 , k_2 are the same as in the model of the thermal decomposition process. These parameters k_1, k_2

are shown in Table 8.3. Next, the change of the soluble matter is considered. Naturally, P is the matter other than A, B and C, and P_{Wt} is the weight of the water and gas produced by oxidation. The model shown in Fig.8.12_a is a simple one considering the reaction paths between each of the variables A, B, C and P. The reaction paths of P to B and C are physically meaningless. Therefore, the model shown in Fig.8.12_a is corrected as shown in Fig.8.12_b. We will discuss this model with respect to the reaction order and the existence of each path. First, the effect of the concentration is considered. Paying attention to the data given by the experiments under the same experimental conditions except for the initial concentration, as say Run 8-1, Run 8-4 and Run 8-5, this data is rearranges by the normalizing technique as shown in Fig.8.13~Fig.8.18. The basis of the normalizing is taken as $B_{Wt,init}$, $C_{Wt,init}$ and $(B_{Wt} + C_{Wt})_{init}$ because we want to get some informations about the existence of each reaction path. From Fig.8.13, Fig.8.15, Fig.8.16, it is assumed that all reaction paths are first order with respect to concentration. This assumption may not be strictly correct, but according to it, the calculation under certain circumstances, for example, when investigating optimal policy, becomes simple. Therefore, we accept this assumption in so far as the first order assumption can explain the experimental data skillfully to some extent. Next, we will discuss whether each reaction path as shown in Fig.8.12_b exists or not. The reaction path from B to C exists because C_{Wt} increases at least once in all cases of the experiments. The question is whether the reaction path from C to B exist or not, or whether the reaction between B and C is reversi-

Table 8.2 Linear regression model.

Linear regression model	
A_{COD} against A_{Wt}	$A_{\text{COD}} = 1.313 \cdot A_{\text{Wt}} + 4080$
B_{COD} against B_{Wt}	$B_{\text{COD}} = 1.018 \cdot B_{\text{Wt}} - 260$
C_{COD} against C_{Wt}	$C_{\text{COD}} = 0.55 \cdot C_{\text{Wt}} + 1080$
C_{Wt} against C_{COD}	$C_{\text{Wt}} = 0.967 \cdot C_{\text{COD}} + 460$

Table 8.3 Values of k_1 , k_2 , ξ .

$k_1 = 0.37 \cdot \exp(-249/T)$ $k_2 = 0.319 \cdot \exp(-500/T)$ $\xi = (-0.00457 T + 2.3230) \frac{A_{\text{Wt, init.}}}{A_{\text{Wt}}}$

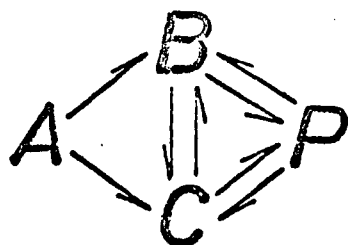


Fig. 8.12_a

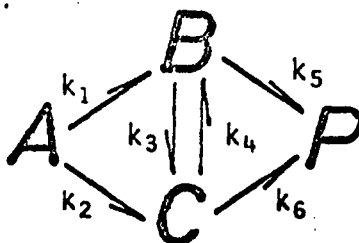


Fig. 8.12_b

Model of the oxidation process.

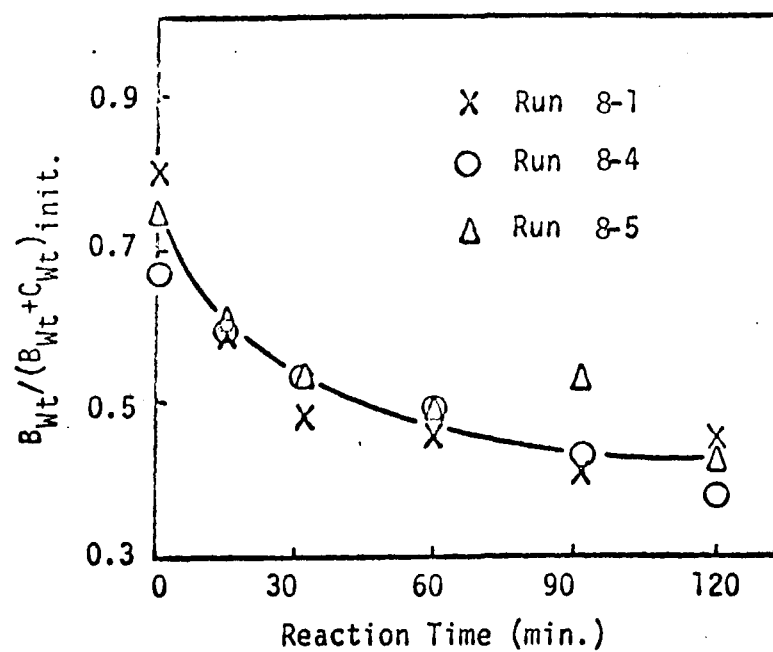


Fig. 8.13 $B_{Wt} / (B_{Wt} + C_{Wt})_{init.}$

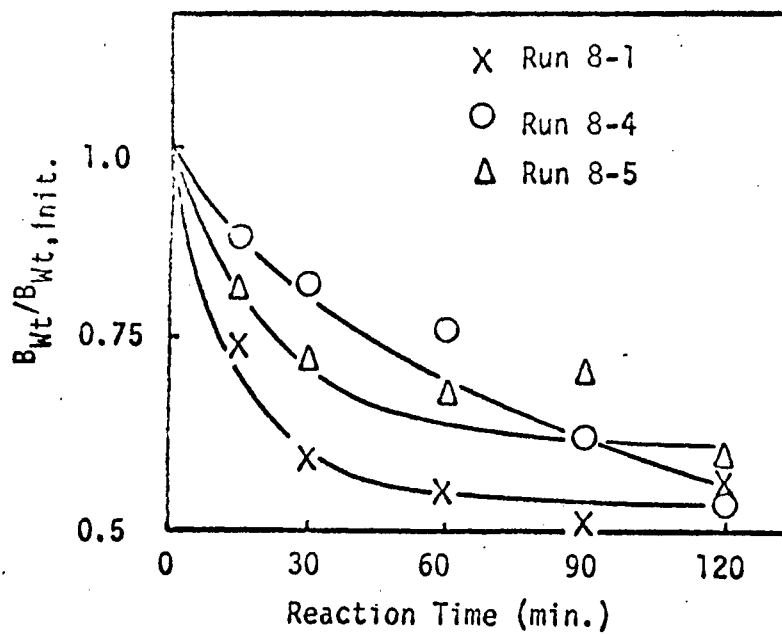


Fig. 8.14 $B_{Wt} / B_{Wt,init.}$

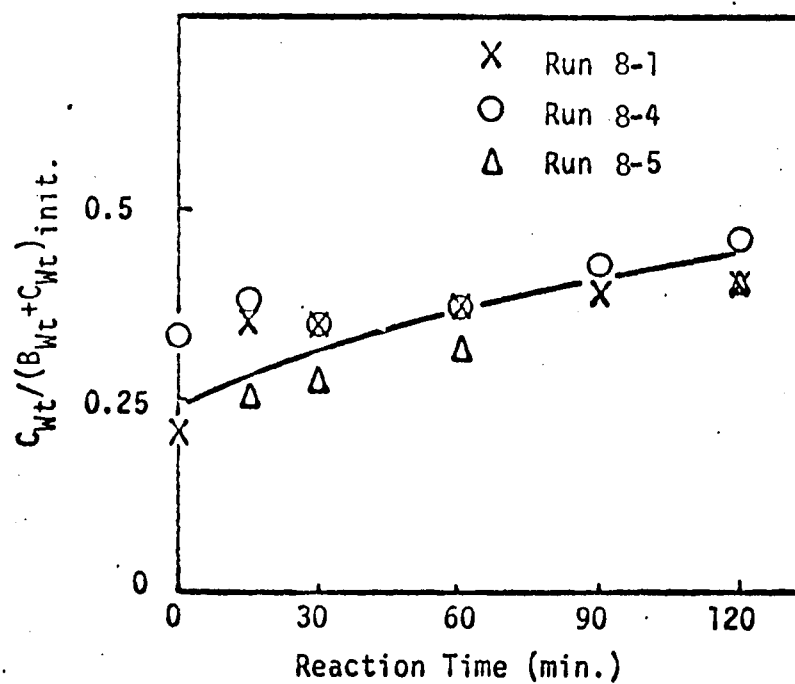


Fig. 8.15 $C_{Wt} / (B_{Wt} + C_{Wt})_{init.}$

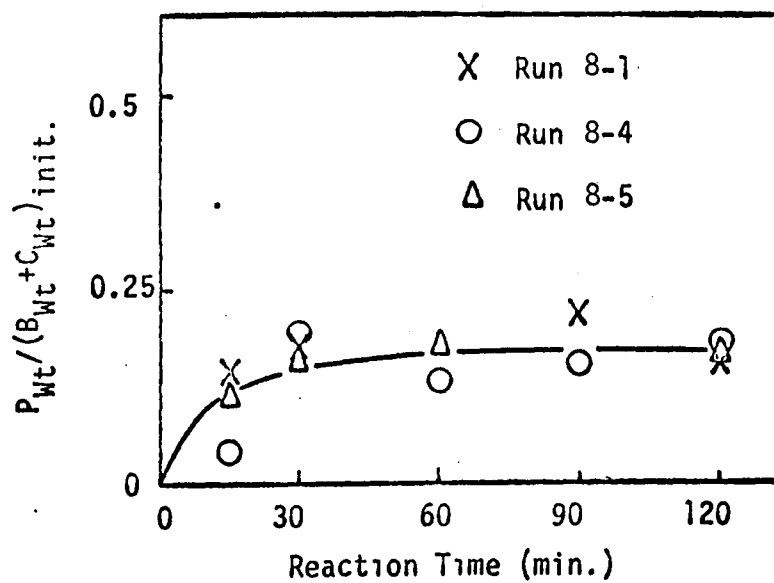


Fig. 8.16 $P_{Wt} / (B_{Wt} + C_{Wt})_{init.}$

ble or irreversible ? If the reaction path from C to B does not exist, the change of $B_{Wt}/B_{Wt,init}$ against time is identical in any case under the same experimental conditions except for $B_{Wt,init}$, for the reactions are all of the first order. As shown in Fig.8.14, this relation with respect to $B_{Wt}/B_{Wt,init}$ is not satisfied. Furthermore, if the reaction order is not first, initial reaction rate $B_{Wt}/B_{Wt,init}$ becomes greater or smaller in order of the initial concentration of B_{Wt} . This condition is not satisfied as shown in Fig.8.14. On the other hand, the value of $B_{Wt}/(B_{Wt}+C_{Wt})_{init}$ changes in the same way as in the cases of Run 8-1, Run 8-4 and Run 8-5. If so, it may be said that the reaction path from C to B exists.

At least one of the reaction paths from B to P and from C to P exists because P is produced in the oxidation process. The existence of P is clear from the analysis of the gas. First, the reaction path from B to P is examined. If this reaction path does not exist, the initial producing rate of P depends only on the initial concentration of C. If this reaction is of the first order, the initial rate of $P_{Wt}/C_{Wt,init}$ is the same value in case where $C_{Wt,init}$ is different. If this reaction is not of the first order, the initial rate of $P_{Wt}/C_{Wt,init}$ becomes greater or smaller according to $C_{Wt,init}$. As shown in Fig.8.17, both conditions mentioned above are not satisfied. So, it can be said that the reaction path from B to P exists.

Next, the reaction path from C to P is examined. The method of examination is similar to examination of the reaction path from B to P. That is to say, the value of $P_{Wt}/C_{Wt,init}$ is used for this examination. From Fig.8.18, it is assumed that the reaction

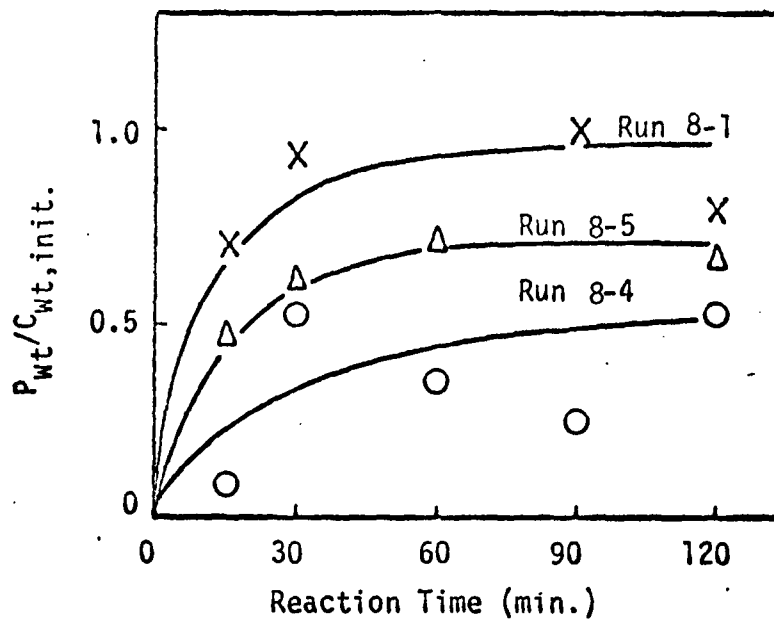


Fig. 8.17 $P_{Wt}/C_{Wt,init.}$

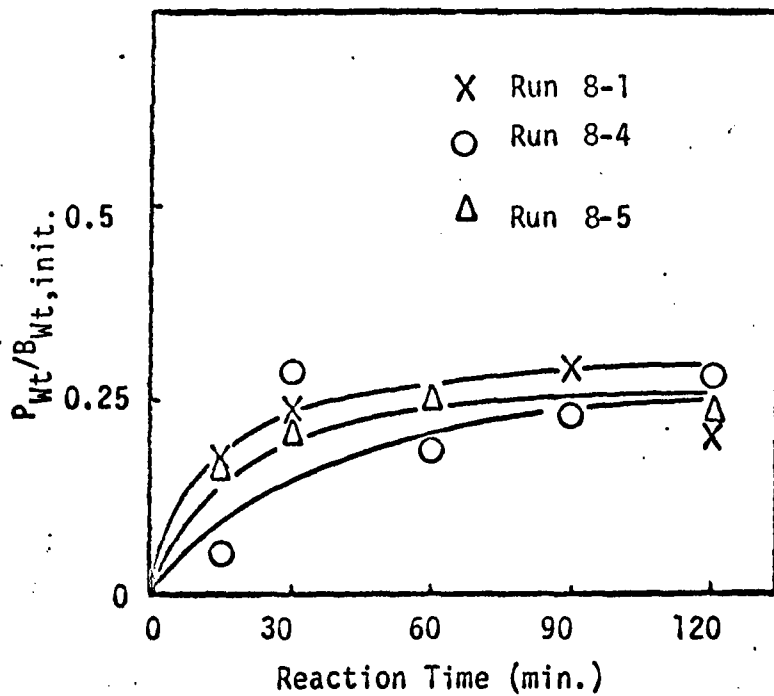


Fig. 8.18 $P_{Wt}/B_{Wt,init.}$

path from C to P exist. However, it is expected that the reaction rate of the reaction path from C to P is small. Finally, it can be said that both reaction paths from B to P and from C to B exist. For the above examination it is assumed that the experimental condition of Run 8-1, Run 8-4 and Run 8-5 are the same except for the initial concentration. But strictly speaking, this assumption is not correct as shown in Fig.8.5. Here, it is assumed that the difference between the assumption and the fact is small. Finally, from the above examination, the model of the oxidation process with respect to the weight becomes one as shown in Fig.8.12b, where the reaction order of all paths is first.

The experimental condition of the total pressure of the reactor does not directly affect the oxidation process but does so indirectly as the thermal decomposition process. We do not consider the effect of the pressure in the model of the oxidation process. Finally, on the assumption of the rate constant being subject to the Arrhenius-type, the mathematical model of oxidation process with respect to the weight becomes as follows :

$$\frac{dA_{Wt}}{dt} = -(k_1 + k_2) \cdot (1 - \xi) \cdot A_{Wt} \quad , \quad (8.1)$$

$$\frac{dB_{Wt}}{dt} = k_1 \cdot (1 - \xi) \cdot A_{Wt} - (k_3 + k_5) \cdot B_{Wt} + k_4 \cdot C_{Wt} \quad , \quad (8.2)$$

$$\frac{dC_{Wt}}{dt} = k_2 \cdot (1 - \xi) \cdot A_{Wt} + k_3 \cdot B_{Wt} - (k_4 + k_6) \cdot C_{Wt} \quad , \quad (8.3)$$

$$P_{Wt} = A_{Wt,init.} + B_{Wt,init.} + C_{Wt,init.} - A_{Wt} - B_{Wt} - C_{Wt} \quad (8.4)$$

where the initial conditions are

$$A_{Wt_{t=0}} = A_{Wt,init} , B_{Wt_{t=0}} = B_{Wt,init} , C_{Wt_{t=0}} = C_{Wt,init} , \quad (8.5)$$

and k_i , ξ are

$$k_i = k_i^0 \exp\left(-\frac{E_i}{R \cdot T}\right) , \quad i = 1, \dots, 6 \quad (8.6)$$

$$\xi = (a \cdot T + b) \frac{A_{Wt,init.}}{A_{Wt}} , \quad (8.7)$$

where k_i^0 is the frequency factor and E_i is activation energy.

The assumption that the rate constant is subject to the Arrhenius-type may be incorrect due to being an oversimplification. But if the experimental data is explained skillfully to some extent by using this assumption, it is not so erroneous. A situation like this may be inevitable during the first stage of model identification.

Finally, the mathematical model of the oxidation process with respect to the weight is represented by Eq.(8.1)~Eq.(8.7). And the COD value of each variable is estimated by using the linear regression model as shown in Table 8.2.

8-6. PARAMETER FITTING

We will estimate the values of the parameters in the mathematical model of the oxidation process with respect to the weight. The values of k_1° , k_2° , E_1 , E_2 , a and b in Eq.(8.1)~Eq.(8.7) have been estimated in the thermal decomposition process, and these parameters values can be used in the mathematical model of the oxidation process as previously mentioned. Then the values of k_i° , E_i ($i=3, \dots, 6$) in Eq.(8.1)~Eq.(8.7) are to be estimated from the experimental data. As the procedure of parameter fitting has already been described in Chapter 7, the same explanation is not mentioned here.

Essentially, C_{Wt} is not observed directly but is estimated by the linear regression model of C_{Wt} against C_{COD} . If it is not assumed that C_{Wt} is the observed value, parameter fitting will be poor, for various combinations of each parameter values of k_3° , k_4° , k_5° , E_3 , E_4 and E_5 satisfy the criterion that the squares of the observation error is minimum. Furthermore the parameter values of k_6° and E_6 cannot be estimated from the observed data B_{Wt} and $(A_{Wt} + B_{Wt})$. Therefore, it is assumed that the predicted value of C_{Wt} given by the linear regression model of C_{Wt} against C_{COD} is the observed value, and that the error of this prediction has a Gaussian distribution with a zero mean and variance of σ^2 . This assumption is necessary for the statistical treatment of parameter fitting. Then, the problem of parameter fitting in this case is described as follows : A set of ordinary differential equations is given in Eq.(8.1)~Eq.(8.7). Then, find the value of parameter θ described

in Eq.(8.11) which minimizes a function such as

$$F(\theta) = \sum_{r=1}^R [y(t_r) - g[x(t_r)]]' \cdot M^{-1} \cdot [y(t_r) - g[x(t_r)]] , \quad (8.8)$$

where "'" denotes the transpose vector, -1 denotes the inverse matrix, M_r is the covariance matrix of error η_r , $y(t_r)$ is the observed value vector at time t_r and g is the observed function vector of state variables.

To solve this problem, the gradient method is used as shown in Chapter 2, 7 and references [8.5],[8.6]. In our problem, $y(t_r)$, g and θ are given as follows,

$$y(t_r) = \begin{bmatrix} A_{wt} + B_{wt} \\ B_{wt} \\ C_{wt} \end{bmatrix} \text{observed value at time } t_r , \quad (8.9)$$

$$g[x] = \begin{bmatrix} A_{wt} + B_{wt} \\ B_{wt} \\ C_{wt} \end{bmatrix} \text{calculated value at time } t_r , \quad (8.10)$$

$$\theta' = (k_3^o , k_4^o , k_5^o , k_6^o , E_3 , E_4 , E_5 , E_6) \quad (8.11)$$

and M_r is taken as

$$M_r = I \cdot \sigma^2 \quad (8.12)$$

where σ^2 is the variation of observation error of the weight and has the value of $6 \times 10^3 [\text{mg/kg-total-sludge}]^2$. When a parameter fitting is performed by using the gradient method, the first assumed values of the parameters are significant. If the first assumed

values are poor, the calculation time of parameter fitting often becomes very long, or that the estimated values of the parameters have no physical meaning. The first assumed values are investigated by using the analog computer ALS-1000, and from the investigated values of the parameters, the calculation is started by the digital computer KDC-II. From the result of this calculation, the fitted parameter values are shown in Table 8.4. The calculated values of each variable resulting from using these estimated parameter values are shown as a solid curve in Fig.3.6_a~Fig.3.11_a. The COD values estimated by using a linear regression model of COD against the weight are shown as a solid curve in Fig.3.6_b~Fig.3.11_b. In these figures, the shaded parts show the 95[%] confidence regions with respect to the expected values.

The mathematical model of the wet-air oxidation process becomes as follows.: The thermal decomposition model with respect to the weight is,

$$\frac{dA_{Wt}}{dt} = -(0.37 \cdot e^{-\frac{249}{T}} + 0.319 \cdot e^{-\frac{500}{T}}) \cdot (1-\xi) \cdot A_{Wt} \quad , \quad (8.13)$$

$$\frac{dB_{Wt}}{dt} = 0.37 \cdot e^{-\frac{249}{T}} \cdot (1-\xi) \cdot A_{Wt} - 1800 \cdot e^{-\frac{4600}{T}} \cdot B_{Wt} + 0.55 \cdot e^{-\frac{1260}{T}} \cdot C_{Wt} \quad (8.14)$$

$$C_{Wt} = (A_{Wt} + B_{Wt})_{init.} - A_{Wt} - B_{Wt} \quad , \quad (8.15)$$

where,

$$\xi = \frac{A_{Wt,init.}}{A_{Wt}} (-0.00457 \cdot T + 2.323) \quad ,$$

and the oxidation model with respect to the weight is,

$$\frac{dA_{Wt}}{dt} = -(0.37 \cdot e^{-\frac{249}{T}} + 0.319 \cdot e^{-\frac{500}{T}}) \cdot (1-\xi) \cdot A_{Wt}, \quad (8.16)$$

$$\frac{dB_{Wt}}{dt} = 0.37e^{-\frac{249}{T}} \cdot (1-\xi)A_{Wt} - (1.41e^{-\frac{3270}{T}} + 120e^{-\frac{4700}{T}})B_{Wt} + 1.94e^{-\frac{5300}{T}}C_{Wt}, \quad (8.17)$$

$$\frac{dC_{Wt}}{dt} = 0.319e^{-\frac{500}{T}} \cdot (1-\xi)A_{Wt} + 1.41e^{-\frac{3270}{T}}B_{Wt} - (1.94e^{-\frac{5300}{T}} + 10.5e^{-\frac{5300}{T}})C_{Wt}, \quad (8.18)$$

$$P_{Wt} = (A_{Wt} + B_{Wt} + C_{Wt})_{init.} - A_{Wt} - B_{Wt} - C_{Wt}. \quad (8.19)$$

The change of the COD value is estimated by the linear regression model of COD against the weight as shown in Table 8.2.

Table 8.4 Fitted parameter values.

$k_3 = 1.14 \cdot \exp(-3270/T)$
$k_4 = 1.94 \cdot \exp(-5300/T)$
$k_5 = 120 \cdot \exp(-4700/T)$
$k_6 = 10.5 \cdot \exp(-5300/T)$

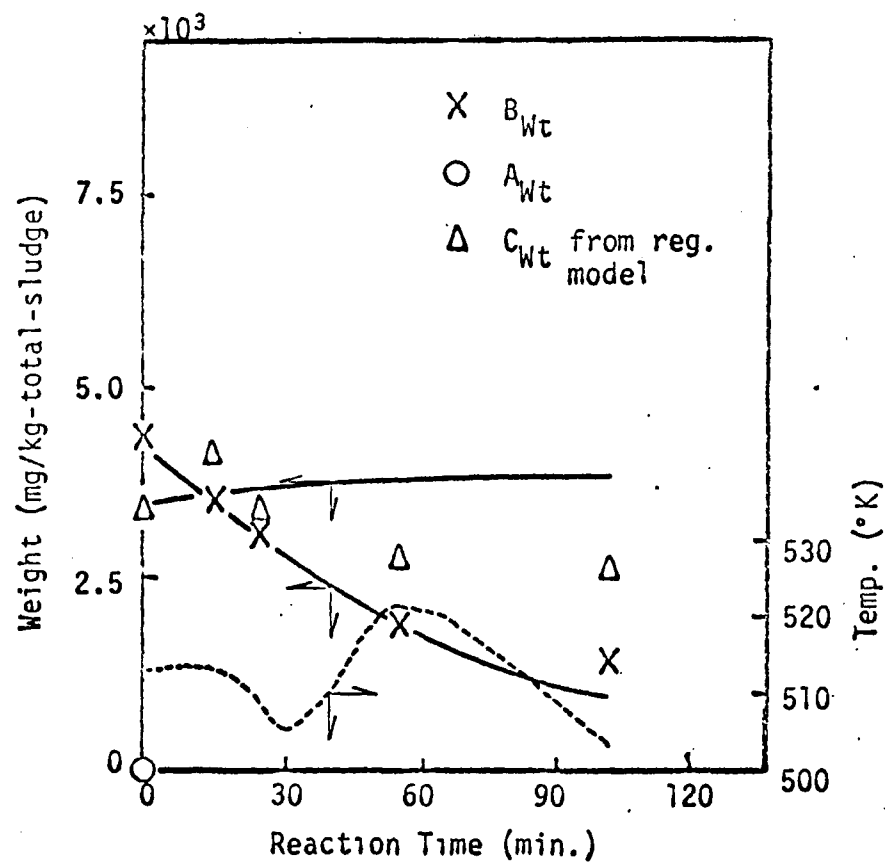


Fig. 8.19 Change of the weight.

8-7. DISCUSSION

It is assumed that the rate constant is subject to the Arrhenius-type and that the reaction path from C to P exists. Based on these assumptions, the mathematical model explains the experimental data fairly well. Thus, it can be said that these assumption are not so erroneous.

Another experiment is performed by using the same sample of artificial cultured activated sludge as previously mentioned. The equipment used in this experiment is the same as above mentioned. The result of this experiment is shown in Fig.8.19. In this figure, the dotted curve indicates the temperature of the reaction. The calculated values resulting from using this model described in Eq.(8.16) Eq.(8.19) are shown as a solid curve. This model too explains the experimental data fairly well.

The analysis of the gas is performed by gas chromatography. The produced gas is composed mainly of CO_2 and partially of CO and other organic gases.

We have used the linear regression model of COD against the weight and model of the weight against COD. These linear regression models are models when only one variable is subject to error. But actually, the observed values of the COD and the weight are both subject to error. When both variables are subject to error, the method examining how to fit a straight line has been reported^[8-7], but the author does not use this situation because the statistical examination of the model is less informative than the case when one variable is subject to error. And it is assumed

that only one variable is subject to error. When we use the linear regression model of COD against the weight, it is assumed that the weight is known deterministically. Concerning the model of the oxidation process, if the time goes to infinity, all the values of A_{Wt} , B_{Wt} , C_{Wt} become zero. It may be said that this does not correspond with reality, but the practical application of this mathematical model is limited with respect to the experimental conditions of time, temperature, concentration, pressure and so on. Thus, when we use this model outside of the limitations, we must take a prudent attitude.

We did not estimate the initial values of the state variables A_{Wt} , B_{Wt} , C_{Wt} . If for example, the initial value of C_{Wt} is estimated by similar manner to parameters k_1 , the experimental data may be more precisely explained.

8-8. CONCLUDING REMARKS

The mathematical model of the oxidation process was proposed based on the experimental data^[8-4], and the parameters of this model were estimated by using the steepest descent method. The volume of oxygen in the reactor was much greater than the theoretical volume calculated by the COD value of the sludge. The effect of the volume of oxygen on the reaction rate was not considered.

NOMENCLATURE

Only the typical nomenclatures are cited.

A ; solid matter

a ; parameter

B ; soluble nonevaporative matter

C ; Soluble evaporative matter

COD ; Chemical Oxygen Demand [mg/l-total-sludge]

k_i ; reaction rate constant

P ; final product in oxidation process

T ; temperature [$^{\circ}$ K]

t ; time [min.]

W_t ; weight [mg/kg-total-sludge]

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CHAPTER 9

RATIONAL DESIGN OF A WASTE WATER TREATMENT SYSTEM

9-1. INTRODUCTORY REMARKS

In this chapter, the method proposed in Chapter 5 is applied to the rational design of a waste water treatment system composed of an activated sludge treatment process from the viewpoint of a systems engineering approach. In this approach, all the subsystems which constitute the waste water treatment system are first represented by a simple mathematical model, partially described in Chapter 8. The total system design investigated in this chapter aims at a decision on the optimum capacity of each unit operation under given conditions of flow rate, and inlet and outlet average concentration. The method of determining a rational design margin to compensate for the undesirable effects on system performance due to the parameter uncertainties proposed in Chapter 5 is applied to determination of the margins of the design variables of a waste water treatment system whose predicted input flow rate involves some error.

9-2. MATHEMATICAL REPRESENTATION OF PROCESS SYSTEM

The mathematical model of each unit operation must represent the relation between the degree of treatment and the size of each unit operation. The total system comprizing an activated sludge process and a sludge treatment system is shown in Fig.9.1. The sludge treatment system is composed of a thickening unit, wet-air oxidation process, dehydrating unit and incinerating unit. The static mathematical model for each unit is given as follows, being developed from experimental studies^{[9-1],[9-2],[9-3]}. In the following equations, the state variables x_1 and x_2 represent BOD₅ and SS concentrations, respectively, of waste water in each unit. Superscripts indicate inputs to or outputs from each unit as shown in Fig.9.1, and V_i is the volume of the unit process i ($i=A, S, T, W$). y is the input flow rate into the total system, and r, w, ϵ and α are the ratios of return flow rate from each unit to the aeration tank.

In an aeration tank, the mathematical model on the assumption of complete mixing is given by

$$V_A \dot{x}_i^1 = (1+r+w+\epsilon)y(x_i^0 - x_i^1) + V_A R_i^1, \quad i = 1, 2 \quad (9.1)$$

where $\dot{x}_i^1$ represents the derivative of x_i^1 with respect to time t .

R_i^1 in Eq.(9.1) are the reaction rates of the substrate and the activated sludge, given by Eq.(9.2) from the experimental study^[9-1]

$$R_1^1 = -kx_1^1 x_2^1 + \beta b x_2^1, \quad R_2^1 = a k x_1^1 x_2^1 - b x_2^1 \quad (9.2)$$

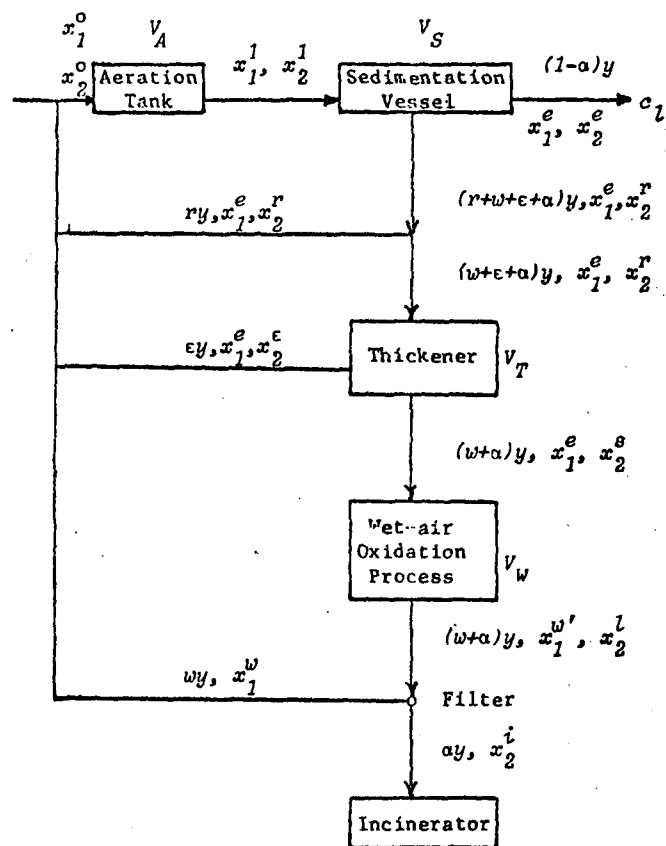


Fig. 9.1 Schematic diagram of waste water treatment system.

where,

α = conversion ratio of substrate to activated sludge
[SSppm/BOD₅ppm]

b = rate constant of decomposition of sludge [1/hr]

k = rate constant of consumption of substrate per unit weight
of activated sludge [1/hr/SSppm]

β = conversion ratio of activated sludge to substrate
[BOD₅ppm/SSppm]

and these parameters can be estimated from experimental data.

Under steady state conditions, the next condition

$$\dot{x}_i^1 = 0, \quad i = 1, 2 \quad (9.3)$$

must be employed.

In a sedimentation vessel, concentration of suspended solid in supernatant liquor x_2^e is represented by a function of sludge concentration in the mixed liquor and retention time as^[9-1]

$$x_2^e = d(x_2^1)^n \exp\left(-A \frac{V_s}{(1+r+w+\epsilon)y}\right) \quad (9.4)$$

where d , n and A are constant parameters. Since it may be natural to assume that the concentration of substrate does not change in the sedimentation vessel,

$$x_1^e = x_1^1 \quad (9.5)$$

The concentration of recirculated sludge x_2^r is represented by an exponential function of retention time

$$x_2^r = C_\infty^r \left\{ 1 - \exp\left(-B \frac{V_s}{(1+r+w+\epsilon)y}\right) \right\} \quad (9.6)$$

where C_{∞}^r is the concentration of sludge for the condition of infinite retention time, and B is a constant given by experimental data.

The mass balance in a sedimentation vessel can be written as

$$(1+r+w+\epsilon)x_2^1 = (r+w+\alpha+\epsilon)x_2^r + (1-\alpha)x_2^e \quad (9.7)$$

In the thickening unit, concentration of sludge to be sent to wet-air oxidation process x_2^s is given in the same way as Eq.(9.6)

$$x_2^s = C_{\infty}^s \{ 1 - \exp(-E \frac{V_T}{(w+\epsilon+\alpha)y}) \} \quad (9.8)$$

where C_{∞}^s and E are constants given by the experimental data. If the return sludge from the thickener to the aeration tank has the flow rate $\epsilon \cdot y$ and the concentration of sludge is x_2^e , the equation

$$(\alpha+w+\epsilon)x_2^r = (w+\alpha)x_2^s + \epsilon x_2^e \quad (9.9)$$

is obtained from the mass balance.

In the wet-air oxidation process, the sludge of concentration x_2^s and flow rate $(w+\alpha)y$ must be treated by oxidation. If the sludge in this oxidation process is divided into three groups such as solid matter A , soluble nonevaporative matter B below 120°C, and soluble evaporative matter C below 120°C, and if the overall weight concentration of the three groups in the reactor are denoted by $x_2^{l,A}$, $x_2^{l,B}$, $x_2^{l,C}$, respectively, the relations among these variables become as follows under the assumption of a complete mixed tank reactor,

$$V_W \dot{x}_2^{l,j} = (w+\alpha)y(x_2^j - x_2^{l,j}) + V_W \dot{R}_j, \quad j=A,B,C \quad (9.10)$$

where x_2^j is the concentration of the j -th group in the input flow

to the reactor. The following conditions are assumed :

$$x_2^A = x_2^S, \quad x_2^B = x_2^C = 0 \quad (9.11)$$

R_j in Eq.(9.10) denotes reaction rates and is represented by the first order triangular reaction^[9-3]

$$\begin{vmatrix} R_A \\ R_B \\ R_C \end{vmatrix} = \begin{vmatrix} -(k_1+k_2), & 0 & 0 \\ k_1 & -(k_3+k_5), & k_4 \\ k_2 & k_3 & -(k_4+k_6) \end{vmatrix} \begin{vmatrix} x_2^{L,A} \\ x_2^{L,B} \\ x_2^{L,C} \end{vmatrix} \quad (9.12)$$

where $k_1 \sim k_6$ are reaction rate constants which vary depending on temperature. At the steady state, the conditions

$$\dot{x}_2^{L,j} = 0, \quad j = A, B, C \quad (9.13)$$

are satisfied in Eq.(9.9). Separation of solid matter A, and soluble matters B and C from the oxidized sludge is so easy that a separation unit for this purpose is not so significant in studying the total system design. In the separation of solid matter A from the oxidized sludge, the condition of

$$x_2^L = x_2^{L,A} \quad (9.14)$$

is realized, and soluble matters B and C contained in the supernatant liquor must be returned to the aeration tank. The values of $x_2^{L,B}$ and $x_2^{L,C}$ have a significant effect on the COD concentration of the return flow, as shown in Eq.(9.15) and as shown in Chapter 7,

$$x_2^{l,B}[\text{CODppm}] = 1.018 \cdot x_2^{l,B}[\text{SSppm}] - 260 \quad (9.15)$$

$$x_2^{l,C}[\text{CODppm}] = 0.55 \cdot x_2^{l,C}[\text{SSppm}] + 1080$$

The COD and BOD₅ concentration of soluble matter in the supernatant liquor can be related by a linear equation from the experimental data^[9-4] as shown in Fig.9.2. BOD₅ concentration $x_1^{w'}$ of the supernatant liquor is given by

$$x_1^{w'} = 0.611x_2^{l,B} + 0.33x_2^{l,C} - 2050 \quad (9.16)$$

Assuming that the sludge from the dehydrating unit contains no soluble matters and that the sludge is dehydrated to water content $\gamma[\%]$, then the equations

$$(w+\alpha)x_1^{w'} = wx_1^w \quad (9.17)$$

$$(w+\alpha)x_2^l = \alpha x_2^i \quad (9.18)$$

$$\gamma = 100 - x_2^i \times 10^{-4} \quad (9.19)$$

are given from the mass balance, where x_2^i is the concentration of the sludge fed into the incinerating unit. In this unit, the sludge of the water content $\gamma[\%]$ must be incinerated.

The junction conditions at the inlet of the aeration tank are given by

$$x_1^o = (x_1^f + rx_1^e + \epsilon x_1^e + wx_1^w) / (1+r+w+\epsilon) \quad (9.20)$$

$$x_2^o = (x_2^f + rx_2^r + \epsilon x_2^e) / (1+r+w+\epsilon) \quad (9.21)$$

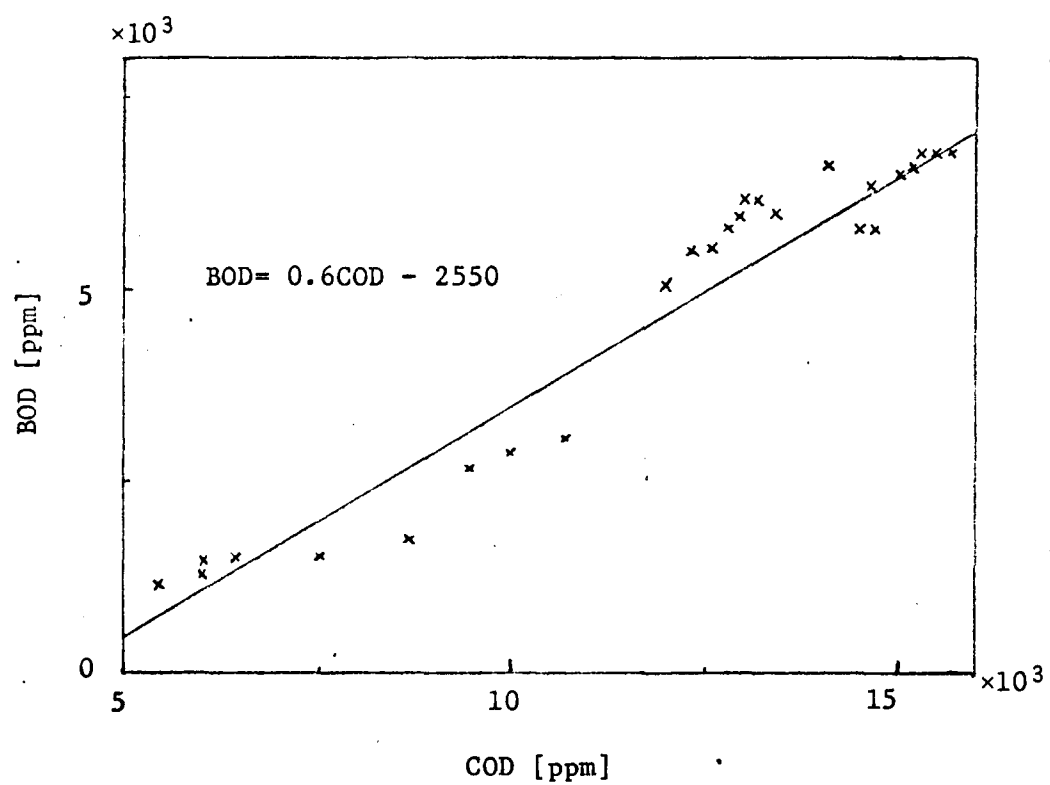


Fig. 9.2 Relation between COD and BOD.

The output concentration of total BOD₅, calculated as the sum of dissolved and suspended matters, is given by

$$C_l = x_1^e + m \cdot x_2^e \quad (9.22)$$

where m is a conversion coefficient of SS to BOD₅. It is desired to fix the value of output BOD₅ C_l at the standard value C_{limit} .

Thus,

$$C_l = C_{limit} \quad (9.23)$$

The equations mentioned above are the process equations and the constraints for design of the total system.

9-3. OPTIMUM DESIGN AT STEADY STATE

In this section, optimum design at steady state is defined as a problem of determining design and operating schemes which minimize the total construction cost of the system illustrated in Fig.9.1 under given input and output conditions. The total construction cost J is provided by

$$J = C_A + C_S + C_T + C_W + C_I + C_P \quad (9.24)$$

where the construction cost $C_i (i=A, S, T, W, I, P)$ [\$] of the unit i is given by

$$C_A = V_A (46.3 + 8120 V_A^{-0.818}) \quad (9.25)$$

$$C_S = V_S (45.0 + 10900 V_S^{-1.126}) \quad (9.26)$$

$$C_T = V_T \{87 + 42 / \exp(V_T / 3720)\} \quad (9.27)$$

$$C_W = 0.41 \times 10^5 V_W \quad (9.28)$$

$$C_I = 1.07 \times 10^5 (\alpha y)^{0.585} \quad (9.29)$$

$$C_P = 7.05 r y \quad (9.30)$$

These are formulated based on results represented in the literature^{[9-5], [9-6], [9-7], [9-8]} as follows.

Construction cost of each unit is given as follows :

Thoes of the aeration tank and sedimentation vessel are given by Eq.(9.25) and Eq.(9.26) from the result of Smith^[9-7] on the base of \$ and m³. Construction cost C_T of the thickener is given by Eq.(9.27)^[9-5]. Construction cost C_W of the wet-air oxidation

process depends on the volume of the reactor as shown in Fig.9.3. This relation is obtained from the data of construction cost^[9-6]. Then, C_W is given by Eq.(9.28). As the dehydrating unit is assumed to weakly depend on the flow rate of the sludge to be dehydrated, construction cost of this unit is considered as a constant cost. The cost of the incinerating unit is a function of flow rate of sludge as given by Eq.(9.29)^[9-8].

The total construction cost can be described by the sum of each construction cost. The decision variables in the system design are the capacity of the unit such as the volumes of the aeration tank, thickener and so on, as well as manipulating variables such as recycle rates. The optimum design to be studied is to determine the values of the decision variables so as to minimize the performance index J given by Eqs.(9.24)~(9.30) subject to the process equations (9.1)~(9.21) and the output conditions of Eqs.(9.22) and (9.23).

Values of the parameters and the boundary conditions used in this calculation are given Table 9.1 and are termed nominal values hereafter. In solving this optimization problem, the steepest descent method is applied.

The results of numerical calculation are shown in Table 9.2. The following becomes evident from the results : i) The plant capacity for the sludge treatment process is much smaller than that of the aeration tank and sedimentation vessel in this solution. For example, the volume of the aeration tank is 7×10^5 times as big as that of the wet-air oxidation process. ii) The retention time in the units calculated are as follows ; $t_A = 4.08[\text{hr}]$, $t_S = 4.37[\text{hr}]$, $t_T = 1.56[\text{hr}]$, $t_W = 4.94[\text{hr}]$. This result shows that the volumes of

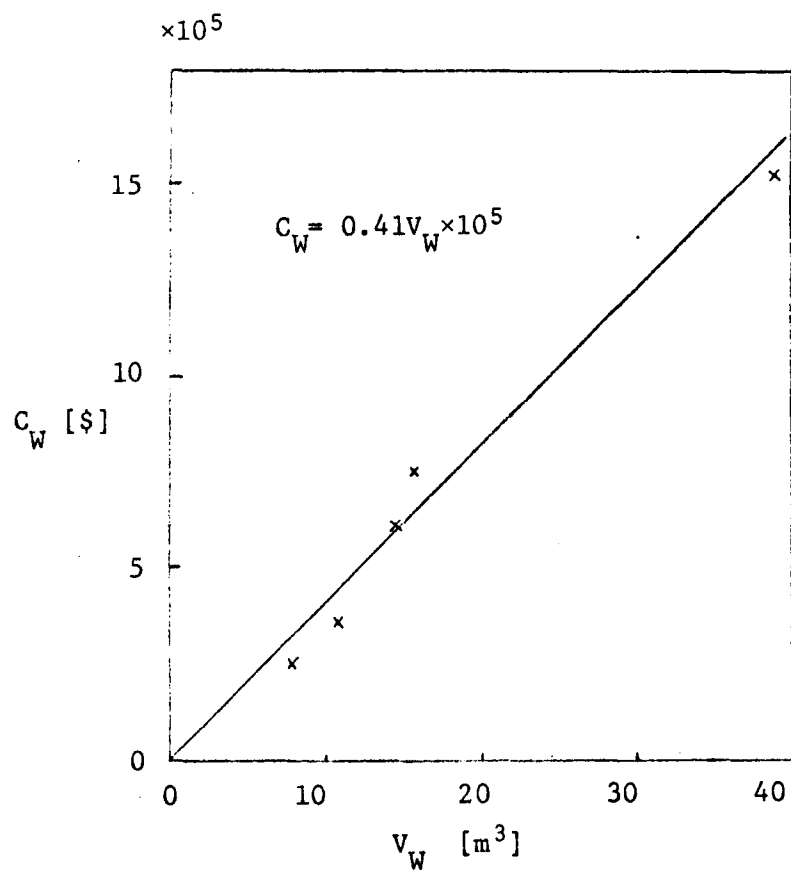


Fig. 9.3 V_W vs. C_W .

Table 9.1 Given parameter values & boundary conditions.

Parameter values	$\alpha=0.52[\text{SSppm}/\text{BOD}_5\text{ppm}], A=0.681[1/\text{hr}], b=0.005[1/\text{hr}]$ $B=E=0.29[1/\text{hr}], C_{\infty}^r=12000[\text{SSppm}], C_{\infty}^B=10^5[\text{SSppm}]$ $d=2.0[(\text{SSppm})^{0.5}], k=0.0005[1/\text{hr}/\text{SSppm}],$ $k_1=13.8[1/\text{hr}], k_2=7.32[1/\text{hr}], k_3=0.162[1/\text{hr}]$ $k_4=0.0054[1/\text{hr}], k_5=0.96[1/\text{hr}], k_6=0.03[1/\text{hr}]$ $m=0.5[\text{BOD}_5\text{ppm}/\text{SSppm}], n=0.5[-], \beta=0.7[\text{BOD}_5\text{ppm}/\text{SSppm}]$
B.C.	$\bar{y}=20000[\text{m/hr}], x_1^f=300[\text{BOD}_5\text{ppm}], x_2^f=0[\text{SSppm}]$ $C_{\text{limit}}=30[\text{BOD}_5\text{ppm}], \gamma=50[\%]$

Table 9.2 Optimum design of total system for nominal values of parameters.

design variable	$\bar{V}_A=1.446 \times 10^5, \bar{V}_S=1.584 \times 10^5$ $\bar{V}_T=179.0, \bar{V}_W=0.198[\text{m}^3]$	per- formance Index $J=1.387 \times 10^7$ (4)
manipulating variable	$\bar{r}=0.765, \bar{w}=2 \times 10^{-6}$ $\bar{e}=5.75 \times 10^{-3}, \bar{\alpha}=1.38 \times 10^{-9}$	
retention time t_i	$t_A=4.08, t_S=4.37, t_T=1.56$ $t_W=4.94$ [hr]	
state variable	$x_1^e=27, x_2^e=6, x_2^r=8621, x_2^1=3757,$ $x_2^B=36320, x_2^e=50, x_1^w=2822, x_2^1=344,$ $x_2^1, B=3551, x_2^1, J=8183, x_2^i=5 \times 10^5$	

both aeration tank and sedimentation vessel are almost equal, which corresponds to a retention time of about 4[hr]. They coincide with the dimensions of plants actually constructed. The value of the concentration of the return sludge x_2^R being about 8600[ppm] also corresponds to the actual design value. iii) The calculated values of the ratios of return flow rates to feed are unrealistic. Especially, the value of $\bar{r}$ is too large when compared with the values of $\bar{\epsilon}$, $\bar{w}$, $\bar{\alpha}$, and yet this result may suggest the effectiveness of the policy to reduce as much as possible the volume of excess sludge to be treated. That is to say, a high rate or the total oxidation method in the activated sludge process may be more desirable than the so-called "conventional method".

9-4. DESIGN MARGIN TO COMPENSATE FOR THE ERROR OF PREDICTED INPUT FLOW RATE

The parameters in a mathematical model involve inevitable estimation errors and may frequently deviate from the nominal values during the operating period. If the actual value of each parameter deviates from the nominal one on which the optimum design has been done, the output value will vary more or less from the optimum state. Usually, some design margins are added to the result from the nominal design to compensate for the undesirable effect of parameter deviations on the system^{[9-10],[9-11],[9-12]}. A method for evaluating design margins quantitatively, taking into account parameter uncertainties, has been proposed by the author and others^{[9-13],[9-14]}. In this section, the extension of the method for more practical use as was proposed in Chapter 5^[9-15] is applied to the design of this system^[9-16].

Generally, in the system design of a sewage treatment process the capacity of each unit is determined based on the flow rate and the concentration of sewage which are estimated from the predicted value of future population. It has been reported that the flow rate of waste water to be treated is proportional to 1.3rd power of population, and that concentration is independent of population^[9-9]. Suppose that the population increases linearly at an increasing rate ζ during the design period T . The rate of population increase usually has some estimation error, and the input flow rate y thus contains an uncertainty. Denoting the error of ζ by v , the un-

certainty Δy of the flow rate calculated from the predicted value of population is given by

$$\Delta y = \{1 + T\zeta(1 + v)\}^{1.3} - \{1 + T\zeta\}^{1.3} \quad (9.31)$$

For example, if $v=0.2$, $T=10$ [year], $\zeta=0.04$ [1/year], the value of Δy is about 12[%].

The problem considered here is to evaluate the design margin $\Delta V_z (z=A, S, T, W)$ to compensate for the effect of the uncertainty of the input y by the method proposed in the previous section.

The numerical values used and the result of the calculation are shown in Table 9.3. As this table shows, the design margins calculated by the method presented in the literature^[9-13], where no account is taken of manipulating variables, have larger values than those in this method. From this calculated result the following is concluded : i) No design margin for the unit operation is required because a small change of the manipulating variable r can sufficiently compensate for the effect of parameter variation. ii) The smaller the allowable range for the change of manipulating variables becomes, the larger the design margin ΔV_S of the sedimentation vessel becomes. From the example, if the allowable ranges of $\Delta r/r$, $\Delta w/w$ and ΔC_L are 1[%], 1[%] and 1[ppm], respectively, there is no need to evaluate the design margin since the undesirable effect of parameter deviation can be compensated for by slightly changing the manipulating variable. iii) It's the sedimentation vessel to which the design margin should be added. This result is suggested by both methods. The value of design margin ΔV_S by the previous method^[9-13] is about 2~4 times more than that by the

Table 9.3 Rational design margin for parameter uncertainty.

range of parameter deviation		allowable range of output ΔC	design margin				
			by the method proposed here	by the previous method			
v	$\Delta y/\bar{y}$		remark	ΔV_S	$\Delta V_A, \Delta V_T, \Delta V_W$	ΔV_S	$\Delta V_A, \Delta V_T, \Delta V_W$
0.2	0.12	$ \Delta C_L \leq 1$	at most at $\Delta r/\bar{r} = 0.0066$ **)	0	$\Delta V_A = \Delta V_T = \Delta V_W = 0$	1.38×10^4	$\Delta V_A = \Delta V_T = \Delta V_W = 0$
0.2	0.12	$\Delta C_L = 0$	at most at $\Delta r/\bar{r} = 0.0111$ ***)	0	"	2.32×10^4	"
0.2	0.12	if allowable $ \Delta C_L \leq 1$, ranges ***) of $\Delta r, \Delta \omega$ are $ \Delta r/\bar{r} < 0.005$ and $ \Delta \omega/\bar{\omega} < 0.005$		3.38×10^3	"	1.38×10^4	"
0.2	0.12	$\Delta C = 0$ if allowable ranges ***) of $\Delta r, \Delta \omega$ are $ \Delta r/\bar{r} < 0.005$ and $ \Delta \omega/\bar{\omega} < 0.005$		1.28×10^4	"	2.32×10^4	"

*) $\Delta \omega$ and Δr are taken as $\Delta \omega = 0, \Delta r = 0$ by the previous method.

**) It is sufficient to compensate for the bad effect of Δy if Δr has that value at most.

***) The case in which controllable ranges $\Delta r, \Delta \omega$ of manipulating variables are given.

present method. iv) The allowable range of the change of the manipulating variable is quite significant in designing the process system.

9-5. CONCLUDING REMARKS

In this chapter, the methodology for rational design of process system was applied to a waste water treatment process. A useful way was presented to decide nominal optimum design, to utilize the uncertainties of parameters for predicting reasonable design margin. On the basis of the methodology given above, the following results are derived concerning the design of waste water treatment systems :

- i) A high rate or total oxidation of the activated sludge process may be more desirable than the conventional method from the viewpoint of reducing construction cost.
- ii) Design margins that compensate for the error of predicted input flow rate are determined rationally. As a result of this, it has been proved that the process systems engineering approach is of great use, even for systems whose parameters contain various kinds and degrees of uncertainty.

NOMENCLATURE

- α ; conversion ratio of substrate to activated sludge
[SSppm/BOD₅ppm]
- A ; parameter in Eq.(9.4) [1/hr]
- C_L ; total BOD₅ of effluent water [BOD₅ppm]
- k ; rate constant of substrate consumption per unit weight of
activated sludge [1/hr/SSppm]
- k_i ; rate constant in Eq.(9.11) [1/hr]
- m ; conversion coefficient from SS to BOD₅ [BOD₅ppm/SSppm]
- r ; ratio of return sludge to input flow rate [-]
- $\bar{r}$; nominal optimum value of r [-]
- Δr ; deviation of r from $\bar{r}$ [-]
- t_i ; retention time of unit i ($i=A, S, T, W$) [hr]
- T ; design period of sewage treatment plant [yr]
- V_i ; volume of unit i ($i=A, S, T, W$) [m³]
- $\bar{V}_i$; nominal optimum value of V_i [m]
- ΔV_i ; design margin of V_i [m³]
- w ; ratio of flow rate from the filtering unit to the aeration
tank [-]
- $\bar{w}$; nominal optimum value of w [-]
- Δw ; deviation of w from $\bar{w}$ [-]
- y ; flow rate of input waste water [m³/hr]
- $\bar{y}$; nominal value of y [m³/hr]
- Δy ; deviation of y from $\bar{y}$ [m³/hr]
- α ; ratio of input flow rate of incinerating unit to feed [-]
- γ ; ratio of water contents [%]
- ϵ ; ratio of flow rate of thickener to aeration tank [-]
- v ; error of rate of population increase [-]
- ζ ; rate of population increase [-]

superscript

e ; output from total system
 f ; input to total system
 i ; input to incinerating unit
 l ; output from wet-air oxidation process
 l,A ; solid matter in oxidized sludge
 l,B ; soluble matter in oxidized sludge
 l,C ; soluble matter in oxidized sludge
 r ; return sludge
 S ; output from thickener to wet-air oxidation process
 w ; output from filter to aeration tank
 w' ; output from wet-air oxidation process
 e ; output from thickener to aeration tank
 0 ; input to aeration tank
 1 ; output from aeration tank
 -1 ; inverse matrix

subscript

A ; aeration tank
 I ; incinerating unit
 P ; pump
 S ; sedimentation vessel
 T ; thickener
 W ; wet-air oxidation process

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CHAPTER 10

RATIONAL DESIGN OF ACTIVATED SLUDGE PROCESS WITH DYNAMIC INPUT DISTURBANCES

10-1. INTRODUCTORY REMARKS

As stated in chapter 4 and 5, it will not always be sufficient to determine the mathematically optimal value based only on a mathematical model, and treatment of parameter uncertainty has been discussed as one of the problems to be considered. In this chapter, a rational static design method for an activated sludge process with dynamic input disturbance will be discussed. This problem is application oriented.

Inputs to the process, that is, the flow rate and concentration of inlet sewage inevitably change in time. They have patterns of daily or seasonal disturbances in a waste water treatment process^[10-1]. Therefore, the size of each unit obtained from the nominal optimum design based on the mean values of the inputs may have to be replaced by the size determined by using the dynamic model. But the data of inputs to be used, if it exists, may increase, or the dynamic nature of an input may be known only as an expected value.

In the customary way of designing plants, mean values of input are used as a basis for determining the capacity of the system, and some margin estimated according to experience is added to this in order to compensate for the dynamic input disturbance.

It may be more practical now to design a waste water treatment process according to the customary method stated above. We must discuss the problem of the relationship between the static design value using a constant input and the value of the dynamic design using dynamic input disturbance that may exist. That is, how does one evaluate the design margin to be added to a nominal static design value? This must be made clear. In this chapter, the problem considered is how the dynamic input disturbance, that is, a time-dependent parameter disturbance, should be taken into account for static system design^[10-8].

10-2. STATIC OPTIMUM DESIGN AND INPUT DISTURBANCE

10-2-1 Mathematical Model of the Process and Static Optimum Design

We consider the activated sludge process illustrated in Fig. 10.1 which is composed of an aeration tank and sedimentation vessel. Process equations are given as follows [10-2].

In the completely mixed aerator

$$V_A \frac{dx_i^1}{dt} = (Y+R) \times (x_i^0 - x_i^1) + V_A R_i, \quad i = 1, 2 \quad (10.1)$$

where R_i represent reaction rate and is given by

$$R_1 = -kx_1^1 x_2^1 + \beta b x_2^1, \quad (10.2)$$

$$R_2 = a k x_1^1 x_2^1 - b x_2^1 \quad (10.3)$$

Parameters a, b, β , and k are constants with respect to the reaction of microorganisms, as shown in Table 10.1. V_A is the volume of the aeration tank [m^3], x_1^i and x_2^i are BOD and SS at station i , respectively. Superscript 0 and 1 represent in flow in to the aeration tank and effluent from the aeration tank, respectively. Y , R and t represent flow rate of the inlet sewage [m^3/hr], flow rate of return sludge [m^3/hr] and time, respectively.

SS and BOD of the supernatant liquid of outlet waste water from the sedimentation vessel are denoted by x_2^e and x_1^e , respectively, and given by the following equations,

$$x_2^e = d(x_2^1)^n \exp\left(-A \frac{V_S}{Y+R}\right), \quad x_1^e = x_1^1 \quad (10.4)$$

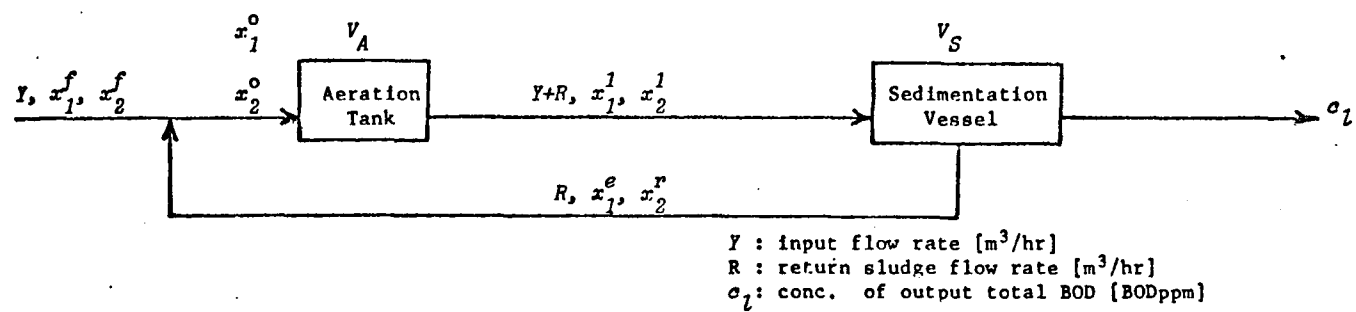


Fig. 10.1 Activated sludge process.

Table 10.1 Given parameter values.

$\alpha = 0.52(\text{SSppm}/\text{BODppm})$	$b = 0.005(1/\text{hr})$
$d = 2.0[(\text{SSppm})^{1/2}]$	$h = 0.681(\text{hr})$
$k = 0.0005[1/(\text{hr} \cdot \text{SSppm})]$	$m = 0.5(\text{BODppm}/\text{SSppm})$
$n = 0.5$	$\beta = 0.7(\text{BODppm}/\text{SSppm})$
$x_1^* = 10,000(\text{SSppm})$	$x_2^* = 0(\text{SSppm})$

where d , n and A are constants given in Table 10.1 and V_s is the volume[m³] of the sedimentation vessel.

At the junction point of recycled activated sludge and input sewage, the following conditions

$$x_i^0 = (x_i^f Y + x_i^r R) / (Y+R), \quad (10.5)$$

$$i = 1, 2$$

are satisfied. We now assume that $x_1^r = x_1^e$. Water quality of effluent waste water is measured as total BOD C_L as follows

$$C_L = x_1^e + m x_2^e \quad (10.6)$$

where m is the conversion coefficient from SS to BOD. Since it is desired to fix C_L at standard value $C_{L\text{limit}}$, the following condition

$$C_L = C_{L\text{limit}} \quad (10.7)$$

must be satisfied. For the steady state

$$\dot{x}_i^1 = 0, \quad i = 1, 2 \quad (10.8)$$

are given in Eq.(10.1).

The nominal static optimum design problem studied here is to determine the optimum volume V_A , V_S of the aeration tank and sedimentation vessel, and the recycle flow rate R which minimize a performance index under a given input Y , x_i^f and output condition $C_{L\text{limit}}$ together with the parameters listed in Table 10.1. The performance index employed here is

$$J = V_A + V_S \quad (10.9)$$

Some examples of the solution of optimal static design for various x_1^f and Y are listed on the left handside of Table 10.2. For example, the solution for $x_1^f = 131.6$, $Y = 3,497.5$ is as follows; $R/Y = 0.6$, $V_A/Y = 3.84$, (hr) $V_S/Y = 4.84$ (hr), where in these numerical calculations $C_{\text{limit}} = 30$ (ppm) is used, and each case in Table 10.2 is explained in 10-2-2. It becomes clear from Table 10.2 that the retention time of each unit (T_A or T_S) becomes small and recycle ration $\gamma \Delta R/Y$ also becomes small when input BOD concentration x_1^f becomes small.

10-2-2 The Effect of Input Disturbance

When inputs having time-dependent disturbances both in flow rate and concentration enter a system which has been optimally design based on the static mean values $x_1^f m$, Y_m , we discuss the effect of input disturbance on the mean values of output total BOD, $C_l m$, from the numerical calculation.

The numerical calculation is made as follows:

Solutions $x_1^e(t)$ and $x_2^e(t)$ which satisfy Eqs.(10.1)~(10.5) based on static optimal design values, $\bar{R}, \bar{V}_A, \bar{V}_S$ and input $x_1^f(t)$ and $Y(t)$ are first calculated. Next, time dependent output $C_l(t)$ can be calculated by the substitution of the solution into Eq.(10.6), and the mean value of $C_l(t)$, $C_l m$ can be determined. Some example of the result are shown on the right handside of Table 10.2.

In Table 10.2, 1-6 is the case where assumed input data is used. In the following numerical examples, case 1-1 to a case 1-5 are the cases where input data is simulated arbitraly in the same way as in case 1-6.

Table 10.2 Optimum design at steady state and effect of input disturbance.

Case	Optimum Design at Steady St.			Effect of Input Disturbance					
	input		optimum design	input				$c_{l,m}$	η
	x_1^f	Y		$x_{1,m}^f$	$x_{1,r}^f$	y_m	Y_{rv}		
1-6	258.6	2.86×10^5	$r=\bar{R}/Y=0.8$ $T_A=\bar{V}_A/Y=6.30$ $T_S=\bar{V}_S/Y=6.251$	258.6	0.207	2.86 10	0.250	31.34	4.5
2	131.6	3497.5	$r=\bar{R}/Y=0.6$ $T_A=\bar{V}_A/Y=3.84$ $T_S=\bar{V}_S/Y=4.84$	131.6	0.231	3497.5	0.198	33.18	10.6
3	81.0	85.7	$r=\bar{R}/Y=0.45$ $T_A=\bar{V}_A/Y=2.76$ $T_S=\bar{V}_S/Y=3.89$	81.0	0.200	85.7	0.168	32.48	8.3

In each case (case 1-1 to case 1-6), mean value of input data is the same value as in the other cases, but the variance of input data is different as we will see when we examine the effect of the variance of input data on output total BOD. Moreover, the pattern of input disturbance has two peaks, one in the morning and evening which corresponds to the actual domestic sewage.

In case 2, input data is taken from actual domestic sewage plants at Kishoin Waste Treatment Plant in Kyoto City. In case 3, input data is given by Eqs.(10.10)~(10.11) which are obtained from the input data taken from Nishiyama Waste Treatment Plant in Nagoya City by the Fourier Series Expansion^[10-3].

That is,

$$\begin{aligned} Y = & 178 - 8\sin x - 72\sin 2x + 5\sin 3x + 8\sin 4x \\ & - 3\sin 5x - 57\cos x - 12\cos 2x + 20\cos 3x \\ & - 7\cos 4x - 3\cos 5x + \cos 6x \end{aligned} \quad (10.10)$$

$$\begin{aligned} x_1^f = & 80 + 3\sin x - 34\sin 2x - 7\sin 3x - 4\sin 4x \\ & + 20\sin 5x - 19\cos x + 10\cos 2x + 4\cos 3x \\ & - 6\cos 4x + 18\cos 5x - 14\cos 6x \end{aligned} \quad (10.11)$$

where x is given by

$$x = \frac{\pi t}{12}$$

where t is time[hr].

Input data in case 1-6, case 2 and case 3 is shown in

Fig.10.2. One example of output $C_L(t)$ is shown in Fig.10.3 in case 2. The values of $x_{1,m}^f$, $x_{1,r\upsilon}^f$, Y_m , $Y_{r\upsilon}$, $C_{L,m}$, η are defined as follows

$$x_{1,m}^f = \frac{1}{T} \int_0^T x_1^f dt, \quad (10.12)$$

$$x_{1,r\upsilon}^f = \frac{1}{T} \int_0^T (x_1^f - x_{1,m}^f)^2 dt / (x_{1,m}^f)^2$$

$$Y_m = \frac{1}{T} \int_0^T Y dt, \quad (10.13)$$

$$Y_{r\upsilon} = \frac{1}{T} \int_0^T (Y - Y_m)^2 dt / Y_m^2$$

$$C_{L,m} = \frac{1}{T} \int_0^T C_L dt, \quad (10.14)$$

$$\eta = (C_{L,m} / C_{\text{limit}} - 1) \times 100$$

That is, $x_{1,m}^f$ and Y_m are mean values of BOD and flow rate, $Y_{r\upsilon}$ and $x_{1,r\upsilon}^f$ are the relative variances of flow rate and BOD, respectively, which represent the degree of distribution of input data.

$C_{L,m}$ is the mean value of output BOD, and η represents the degree of deviation of $C_{L,m}$ from standard or fixed value, C_{limit} .

T in Eqs.(10.12)~(10.14) is taken as follows; $T = 168$ [hr] for case 1-1 ~ case 1-6, $T = 72$ [hr] for case 2, and $T = 48$ [hr] for case 3.

From Table 10.2, the following become clear: When inputs having time-dependent disturbances (mean values are $x_{1,m}^f$, Y_m) enter a system optimally designed based on $x_{1,m}^f$ and Y_m , mean values of output, $C_{L,m}$ don't coincide with C_{limit} which is the fixed value of static optimum design. This fact may be explained as the result of nonlinearity of

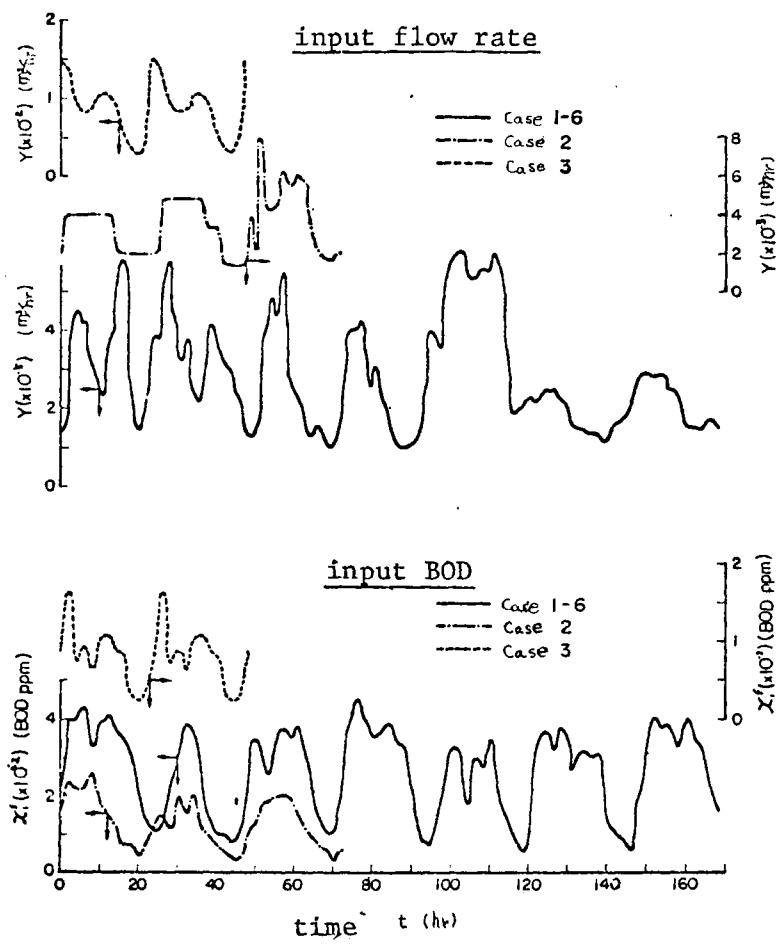


Fig. 10.2 Input data of x_1^f and Y .

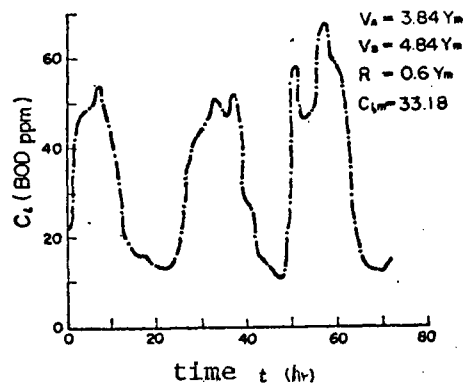


Fig. 10.3 Calculated output C_1 for case 2.

output, because, if there is no effect of input dynamic disturbance on the output variable, $C_{L,m}$ has to be equal to C_{limit} .

If the relative variance of the input flow rate, Y_{rv} , is the same degree in some cases, the effect of nonlinearity on output, which may be represented quantitatively by η in Table 10.2, becomes stronger as the mean value of input BOD, $x_{1,m}^f$ becomes smaller. For example, in case 2, η is about 11%. On the contrary, in case 1-6,

is about 5%. This result is explained as follows: The optimal tank volume becomes small as input x_1^f becomes small, while each tank also has the role of buffer tank against input disturbance. Then, the effect of input disturbance becomes larger when tank volumes are small. These facts explain the results. Naturally the degree of the relative variance of input, Y_{rv} , $x_{1,rv}^f$ gives some effect on η , however, the effect is relatively smaller than the effect of x_1^f . This becomes clear by comparing each case in Table 10.2. The effect of Y_{rv} , $x_{1,rv}^f$ will be discussed in the next section.

As shown in Table 10.2, when static optimal design was performed based on the mean value of the input, the mean values of total output BOD in this system for input disturbance is 5-11% greater than the given fixed value C_{limit} . Optimum design at an unsteady state or design margin taking into account input disturbance may have to be considered.

10-3. OPTIMUM DESIGN AT AN UNSTEADY STATE

We design optimally taking into account input time-dependent disturbance, $x_1^f(t)$ and $Y(t)$. The design may be performed by minimizing J in Eq.(10.9) under the conditions of Eqs.(10.1)-(10.6) and $C_{l,m} = C_{limit}$. There may be much data of $Y(t)$ and $x_1^f(t)$, or it may not be given beforehand while mean values and variance may be expected beforehand. Then, some modification must be considered.

We consider three cases.

- (i) To use explicit functions of $t, x_1^f(t), Y(t)$:

First, we represent time-dependent inputs as explicit functions $x_1^f(t), Y(t)$ based on given data or experience by using some technique, for example, Fourier Series analysis. For example, time dependent inputs may be represented by Eqs.(10.10),(10.11).

Next, optimal design at an unsteady state can be performed based on $x_1^f(t), Y(t)$ and Eqs.(10.1)-(10.6). Parameters included in explicit functions of time $t, x_1^f(t)$ and $Y(t)$ may have uncertainty, and if so, then the design margin can be evaluated if necessary.

- (ii) Using the static model:

Design values are determined based on the static model which is represented by Eqs.(10.1)-(10.6) and (10.8) and given numerous input data.

Input data to be used for calculation may be too much to calculate.

- (iii) To use the static model and mean value,

We calculate the static optimum design value based on the static model and mean values of input data, and we evaluate the design margin to be added to the nominal optimum design value taking into account input disturbance.

Method (i) or (iii) may be more practical: By method (i) we evaluate design margin to be added to the optimal design value based on the dynamic model. The method of evaluating design margin has been given already by the author and others^{[10-4],[10-5]}. Method (iii) is discussed in section 10-4. In this section optimal design based on both dynamic and static models were discussed.

10-3-1 Optimal Design Based on a Dynamic Model and Input;

When inputs $Y(t)$ and $x_1^f(t)$ are given, optimal design values based on the dynamic model are calculated, and the effect of the relative variance of Y and x_1^f on the design values are determined. In this dynamic model, the output total BOD is fixed as a mean value. Thus,

$$C_{1,m} = C_{\text{limit}} \quad (10.15)$$

Optimal design values are given by minimizing J in Eq.(10.9) under the conditions of Eqs.(10.1)-(10.6), (10.14),(10.15). Some examples of the results of numerical calculation are shown in Table 10.3. When the time-dependent input, $x_1^f(t)$ and $Y(t)$ enter an optimally designed system based on a static model, the $x_{1,m}^f, Y_{m,n}$ in Eq.(10.14) which represents the deviation of the output mean value from the desired value are also shown on the right handside of Table 10.3. In Table 10.3, case 1-6, case 2 and case 3 correspond to the ones

Table 10.3 Optimum design based on dynamic model.

case	input				dynamic opt. design				static opt. design	
	x_1/Y_m	Y_m	$x_1 f_{r,v}$	$Y_{r,r}$	R/Y_m	V_A/Y_m	V_S/Y_m	J/Y_m	η	
1-1	258.6	2.86×10^3	0.091	0.019	0.80	6.30	6.25	12.55	-0.10	
1-2			0.091	0.074	0.80	6.50	6.10	12.60	0.46	$\bar{R}/Y_m=0.80$
1-3			0.091	0.250	0.85	6.80	6.20	13.00	3.68	$\bar{V}_A/Y_m=6.30$
1-4			0.207	0.019	0.80	6.30	6.21	12.50	-0.26	$\bar{V}_S/Y_m=6.251$
1-5			0.207	0.074	0.80	6.50	6.13	12.63	0.56	$\bar{J}/Y_m=12.551$
1-6			0.207	0.250	0.85	6.80	6.30	13.10	4.46	
2	131.6	3497.5	0.231	0.198	0.60	4.70	4.90	9.60	10.6	$\bar{R}/Y_m=0.60$ $\bar{V}_A/Y_m=3.84$ $\bar{V}_S/Y_m=4.84$
3	81.0	85.7	0.200	0.168	0.45	3.00	3.99	6.99	8.3	$\bar{R}/Y_m=0.45$ $\bar{V}_A/Y_m=2.76$ $\bar{V}_S/Y_m=3.89$

in Table 10.2.

The following becomes clear from Table 10.3:

- i) If the relative variance of input flow rate, Y_{rv} is the same in some cases, the ratios of the value of design variables V_A , V_S to static optimal value $\bar{V}_A$, $\bar{V}_S$, $V_A/\bar{V}_A$ and $V_S/\bar{V}_S$ becomes greater as the mean value of input BOD, $x_{1,m}^f$ becomes smaller. For example, in case 1-6, V_A is an overdesign of 8% compared with $\bar{V}_A$, however in case 2, V_A is about 22% over designed compared with $\bar{V}_A$. This fact corresponds to the effect of input disturbance to output, and the reason has been described in 10-2-2.
- ii) If the relative variance of input BOD, $x_{1,rv}^f$ is the same value in some cases, the design margins to be added to $\bar{V}_A$ and $\bar{V}_S$ become greater as the relative variance of input flow rate, Y_{rv} becomes greater. For example, in case 1-5, V_A is about 0.5% overdesigned compared with $\bar{V}_A$, however in case 1-6, V_A is about 8% overdesigned. In the same way, if Y_{rv} is the same value, the design margins become greater as $x_{1,rv}^f$ becomes greater. This may be natural and becomes clear from cases 1-3 and 1-6.
- iii) By comparing case 1-3, it may be clear that the 0.12 increase of $x_{1,rv}^f$ requires a 0.5% design margin and that the 0.18 increase of Y_{rv} requires about a 4% design margin. Then the design margin taking into account the input dynamic disturbance depends more on the variance of Y than the variance of x_1^f . This result may be explained from following fact; when Y and x_1^f have positive and negative step changes, the absolute value of the response of the output C_1 more straightly depends on positive

step changes. Step change x_1^f has the opposite effect.

- iv) From the result of cases 1-1 and 1-4, it becomes clear that the optimal design based on the dynamic model is under designed compared with the static optimal design. It is desired that the input having appropriate dynamic disturbance enter the activated sludge process with the object of making the total volumes of each unit as small as possible. That is, the optimal input may be expected to exist^[10-6].
- v) It may not be necessary to change the sludge return ratio R/Y_m if we design based on the dynamic model and dynamic input.
- vi) Roughly speaking, an appropriate design margin may have to be added not to the sedimentation vessel, but only to the aeration tank when we take into account the dynamic input disturbance in the design margin. This fact coincides with the result of the evaluation of design margin in section 10-4.

10-3-2 Optimal Design Based on Static Model and Dynamical Input;

We will calculate the value of the optimal design based on static model and dynamic input data in order to compare it with the optimal design based on the dynamic model. The solution can be calculated by minimizing J in Eq.(10.9) under the conditions of Eqs.(10.1)-(10.6), (10.8) and (10.14). Some results of the numerical calculations are listed in Table 10.4, the difference between the result of the optimal design based on the static model and that based on the dynamic model may be negligible. Small differences exist only in the volume of the sedimentation tank. Then, using the static model instead of the dynamic one, it may be sufficient to

Table 10.4 Optimum design based on static and dynamic model.

case	dynamic model				static model			
	R/Y_m	V_A/Y_m	V_S/Y_m	J/Y_m	R/Y_m	V_A/Y_m	V_S/Y_m	J/Y_m
1-3	0.85	6.80	6.20	13.00	0.85	6.80	6.33	13.13
1-6	0.85	6.80	6.30	13.10	0.85	6.80	6.41	13.21
3	0.45	3.00	3.99	6.99	0.50	3.20	4.11	7.31

design the activated sludge process with a dynamic input. As discussed, however, input data to be used for calculation may be too much to calculate.

10-4. RATIONAL DESIGN MARGIN ACCOUNTING FOR DYNAMIC INPUT DISTURBANCE

As stated in section 10-3, method (i) using dynamic model and the explicit function of t , $Y(t)$ and $x_1^f(t)$ or method (ii) using a static model and mean value has practical meaning for designing an activated sludge process. In this section, we consider method (iii). Let's evaluate the design margin to be added to the nominal design value calculated based on the static model and mean value of input data taking into account the dynamic input disturbance.

The method of evaluating design margin has already been described in Chapter 4^{[10-4],[10-5]}. Here, we will employ Method IV described in Chapter 4 because the calculation by it is simpler.

The design margin is evaluated by using Eqs.(4.60)-(4.61) or (5.6) ~ (5.8) so as to compensate for the input disturbance, where the deviation of the manipulating variable from the static optimum value is disregarded in using Eqs.(4.60) and (4.61).

Now, variance of input data can be used for determining the ranges of parameter deviations which are utilized for determining the design margin, because variance explains the grade of the distribution of the input data. Parameter deviations Δx_1^f , ΔY are assumed to be given by

$$\frac{\Delta x_1^f}{x_{1,m}^f} = \xi \delta x_1^f \quad (10.16)$$

$$\frac{\Delta Y}{Y_m} = \xi \delta Y \quad (10.17)$$

$$\delta x_1^f = (x_{1,rv}^f)^{\frac{1}{2}}, \quad \delta Y = (Y_{r,v})^{\frac{1}{2}} \quad (10.18)$$

where $x_{1,rv}^f$ and Y_{rv} are relative variances of x_1^f and Y , and ξ is an arbitrary constant. Now h in Eq.(4.61) is replaced by ϕ in Eq.(5.8) and represents the increment of J in Eq.(10.9) by adding margins ΔV_A and ΔV_S .

Thus,

$$\phi = \Delta V_A + \Delta V_S \quad (10.19)$$

Considering the deviation of output total BOD C_L , it is desired that ΔC_L be less than ΔC ($\Delta C \geq 0$). Thus

$$\Delta C_L \leq \Delta C \quad (10.20)$$

Finally, rational design value accounting for dynamic input disturbance can be determined by the following procedure: First, the nominal static optimum design values $\bar{V}_A$, $\bar{V}_S$, $\bar{R}$ are calculated based on the mean values of input, $x_{1,m}^f$ and Y_m . Next, the relationship between design margins ΔV_A , ΔV_S , input disturbances Δx_1^f , ΔY and deviation of output BOD, ΔC_L can be calculated by using sensitivity equations, for example, in the same form as Eq.(4.19) or Eq.(5.6). By using this relationship and Eqs.(10.16)~(10.18), (10.20), ΔV_A , and V_S are determined so as to minimize ϕ in Eq.(10.19).

Finally, rational design values, V_A , V_S and R , are taken as $V_A = \bar{V}_A + \Delta V_A$, $V_S = \bar{V}_S + \Delta V_S$, $R = \bar{R}$.

As ξ and ΔC are arbitrary constants, we must determine these values. The values of ξ and ΔC may be predicted the following numerical calculations.

By this method, design margins are determined for various ξ and ΔC . The results are shown in Table 10.5. For the judgement of effectiveness of this method, optimum design by dynamic model and

Table 10.5 Design margin for input disturbance.

	$\Delta V_S=0, \Delta V_A(\%)$						Opti. design by dynamical model	
NC	0			2.0				
ξ	0.1	0.2	0.5	0.1	0.2	0.5	$\Delta V_A(\%)$	$\Delta V_S(\%)$
Case 1-3 $\delta x_1^f=0.302, \delta y=0.50$	9.6	19.2	48.0	0	8.4	37.5	8.0	-0.8
Case 1-6 $\delta x_1^f=0.456, \delta y=0.60$	12.1	24.2	60.5	1.3	13.4	49.8	8.0	0.7
Case 3 $\delta x_1^f=0.447, \delta y=0.41$	10.1	20.2	50.5	0	9.4	39.7	8.7	2.5

input is also shown in Table 10.5. The values ΔV_A and ΔV_S in the 8th and 9th columns in Table 10.5 indicate the values yielded by subtracting the design values by nominal static design from that determined by dynamic optimum design.

For example, in case 1-3, design margins are given by $\Delta V_A = 9.6(\%)$, $\Delta V_C = 0$ at $\xi = 0.1$, $\Delta C = 0$, that is a 9.6% design margin must be added to the design value of the aeration tank only. On the other hand, $\Delta V_A = 8(\%)$, $\Delta V_S = -0.8(\%)$ for the dynamic optimum design. It may be said that the method for evaluating design margin described here is rational. A design margin is added to the aeration tank only because the method for evaluating design margin utilizes an L.P. problem as described in Chapter 4.

Moreover, it may be sufficient to give $\xi = 0.1$ and $\Delta C = 0$ for the method used to estimate the design margin by Eqs.(10.16)-(10.18). It has become clear that the method described in this section is sufficiently practical to design taking into account the input dynamic disturbance.

10-5. CONCLUDING REMARKS

The rational static design method for an activated sludge process with dynamic input disturbance has been proposed and proven to be practical. We assume that model parameters and structure do not change with the dynamic input disturbance and that total output BOD C_L can be evaluated as a mean value. These assumptions, however, may have to be discussed in the future^[10-8].

NOMENCLATURE

α ; conversion ratio of substrate to activated sludge [SSppm/BODppm]

A ; parameter [1/hr]

C_L ; total BOD of effluent water [BODppm]

k ; rate constant of substrate consumption per unit weight of
activated sludge [1/hr/SSppm]

m ; conversion coefficient from SS to BOD₅ [BODppm/SSppm]

V_i ; volume of unit i ($i=A,S$) [m^3]

$\bar{V}_i$; nominal optimum value of V_i [m^3]

ΔV_i ; design margin of V_i [m^3]

Y ; input flow rate [m^3]

ΔY ; deviation of Y from $\bar{Y}$ [m^3]

superscript

f ; input to total system

r ; return sludge

0 ; input to aeration tank

1 ; output from aeration tank

-1 ; inverse matrix

subscript

A ; aeration tank

S ; sedimentation vessel

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SUMMERIZED CONCLUSION

In this paper, some problems of system identification and the realization of optimal systems with parameter uncertainty are studied as follows having the purpose of the synthesis in mind.

In Chapter 1, studies on model building and the application of sensitivity analysis to system synthesis with parameter uncertainty are briefly surveyed. In Chapter 2, parameter estimation by the least square technique is discussed when the model structure is given, and the geometical meaning of the parameter estimation is indicated. In Chapter 3, a method of determining the experimental condition based on estimation error of parameters is presented. And a method of evaluating the rational design margin taking into account parameter uncertainty is proposed and discussed. Moreover, various methods of design rationally taking into account parameter uncertainty are classified and discussed. In Chapter 5, an attempt to design a process system with parameter uncertainty by considering the movable range of manipulating variables is studied. Chapter 6 serves as an introduction to waste water treatment system design. In Chapter 7 and 8, models of the wet-air oxidation process of sludge which may be subsystem of the waste water treatment system are determined and discussed experimentally using the result of

Chapter 2. In Chapter 9, the rational design of a waste water treatment system is tried based on a mathematical model and the results of Chapter 4 and Chapter 5. In Chapter 10, the problem of time-dependent disturbance of input in an activated sludge system is discussed from the viewpoint of the static design of the system.

The main problem in this paper is the treatment of parameter uncertainty in process system design having the purpose of system synthesis in mind. The methodologies and those applications to a waste water treatment system described in this paper may show that those considerations are effective.

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