OPTIMIZATION STUDIES OF ACTIVATED SLUDGE AND REVERSE OSMOSIS WATER PURIFICATION PROCESSES

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by

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PART I

ANALYSIS AND OPTIMIZATION OF STEP AERATION ACTIVATED SLUDGE PROCESS

CHAPTER I

INTRODUCTION

1. BIOCHEMICAL ENGINEERING AND CHEMICAL ENGINEERING

Various definitions of biochemical engineering have been given. H. Hartley (1)* has said that "Biochemical engineering is the practical application of our knowledge of micro-organism. The industrial application of a biochemical process is a combined operation in which the biochemist, the microbiologist, the geneticist, and the chemical engineer are all intimately concerned." In lectures on biochemical engineering at the University of Tokyo in 1963, the following definition has been offered. "Biochemical engineering is that activity concerned with economic processing of materials of biological character or origin to serve useful purposes. The function of the biochemical engineer is that of translating the knowledge of the microbiologist and the biochemist into a practical operation."

From the foregoing definition, it is obvious that biochemical engineering is intimately related to chemical engineering. A biochemical engineer must not only have an appreciation of the biological science, but he also must be well grounded in chemical engineering principles.

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*Numbers in parentheses refer to references given on page 143.

2. OBJECTIVES IN WASTE WATER TREATMENT AND ITS PROCESSES

Municipal and industrial wastes are treated to protect public health, to avoid nuisance, to prevent the polluting of natural water and of industrial water, and to avoid damage suits. The pollutional characteristics of waste waters may be classified according to their state (suspended, colloidal, and dissolved) and their nature (inorganic, organic, gases, and living organisms). However the major components of organic wastes are usually the suspended solids and the organic content. The treatment of this waste is usually carried out in four steps, viz. pretreatment, biological oxidation, sludge treatment, and disposal.

Pretreatment includes screening, grit removal, and sedimentation or flotation. Biological oxidation is usually accomplished in either fixed-bed units (trickling filters) or in fluid-bed systems (activated sludge). It is employed in removing the colloidal and dissolved organic matter and it also plays the most important role in waste treatment. Sludge from the foregoing units requires further treatment, digestion and dewatering before disposal. Let us consider a complete treatment plant as shown in Figure 1. Generally, the activated sludge process is a part of such a plant. The primary settling tank removes settleable solids from the raw waste stream. The settled solids are diverted for stabilization, often by anaerobic digestion. The waste stream from

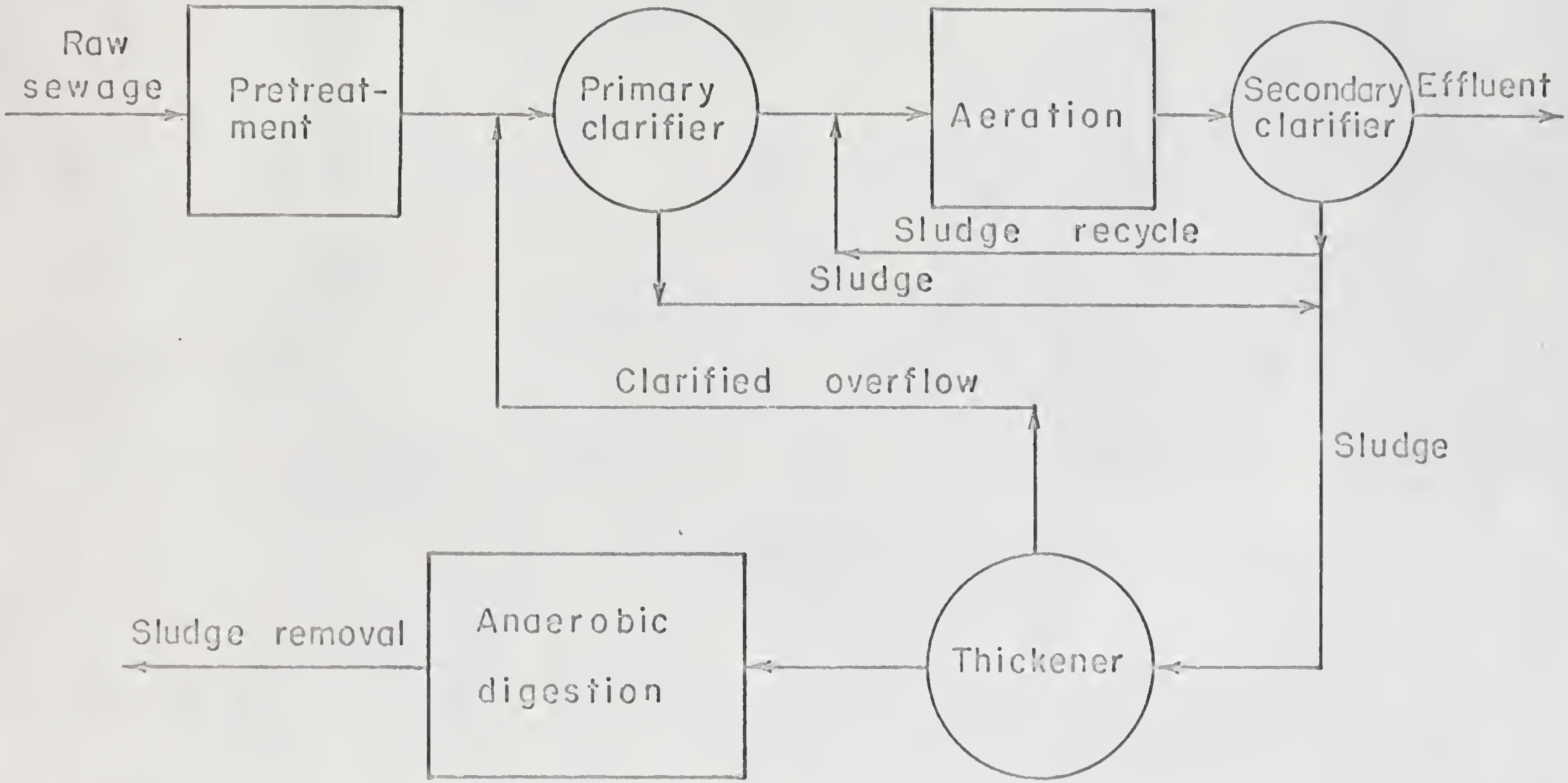


Fig. 1. Activated sludge system with waste disposal by anaerobic digestion.

primary settling enters the aeration phase where the organic matter becomes the food source for aerobic microorganisms. The organisms convert a part of the total food energy to biological cell mass (this is the synthesis step) which remains in the liquid stream leaving the aeration tank. The remaining fraction of the total food is utilized by the organisms as a source of energy for cell synthesis and maintenance. The latter fraction of the food is converted to carbon dioxide and water. The settleable biological solids and inerts are removed from the waste stream in the final settling tank. A part of this activated sludge is returned to the aeration tank to maintain a favorable biological solids concentration in it. The excess solids must be stabilized further, often by anaerobic digestion.

3. ACTIVATED SLUDGE PROCESS

The activated sludge process may be defined as a system in which flocculated biological growths are continuously circulated and contracted with organic waste in the presence of oxygen. The oxygen is usually supplied from air bubbles injected into the sludge-liquid mass. The process involves an aeration step followed by a solid-liquid separation step from which the separated sludge is recycled back and mixed with the incoming waste. A portion of this sludge is removed for further treatment and disposal. The aeration step may be considered in three functional phases as follows (2):

(a) A rapid adsorption of waste substrate by the activated sludge.

(b) Progressive oxidation and synthesis of the absorbed organics.

(c) Further aeration resulting in oxidation and dispersion of the sludge particles.

Various modifications of the activated sludge process have been developed to achieve economic advantage in construction and operation (3). The conventional activated sludge process as shown in Figure 2 is one of the basic activated sludge processes. The present knowledge concerning the treatment has been summarized very effectively by Haseltine (4). According to his report, there are some limitations to this process. In order to overcome the disadvantages of the process, some modifications of the conventional process have been proposed. The step aeration system as shown in Figure 3, developed by Gould (5), is one of the modifications. In essence, the modified process involves the feeding of the sewage flow at different points along the aeration basin. The organic load is thus distributed over the length of the basin. As a result, accelerated growth and oxidation are not confined to one end of the basin as in the conventional process but, instead, take place over most of the basin. The difference between the oxygen demand patterns of the conventional aeration and step aeration is illustrated in Figures 3 and 4.

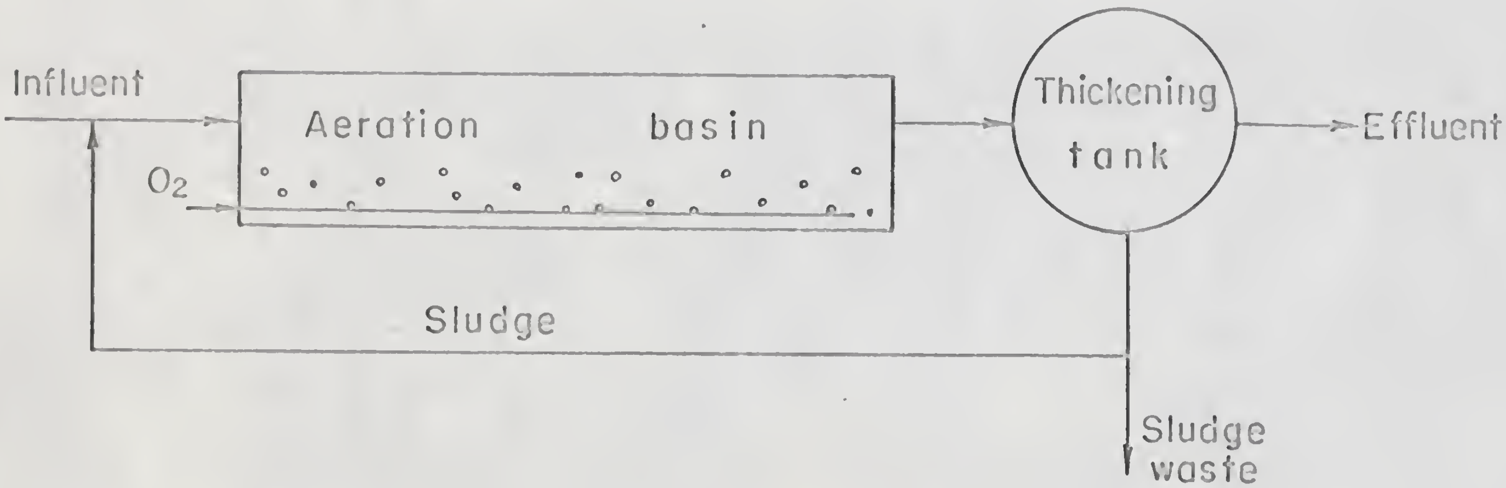


Fig. 2. Flow diagram of conventional activated sludge process.

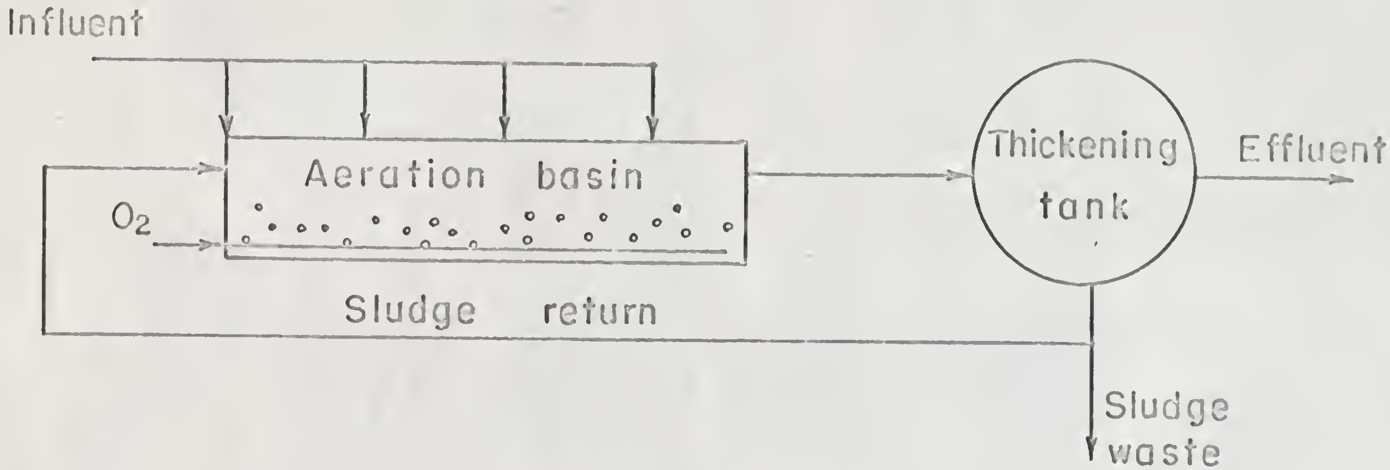


Fig. 3. Flow diagram of step aeration process.

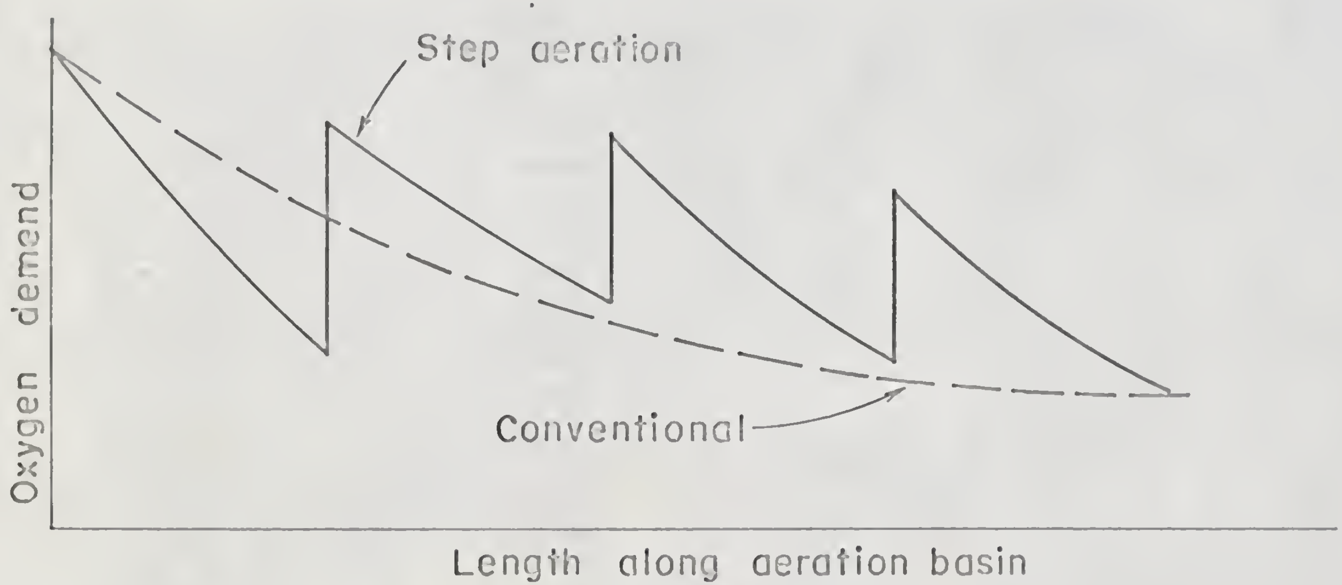


Fig. 4. Comparison of oxygen demands exerted in the conventional and step aeration processes.

4. PROCESS DESIGN AND ECONOMICS

Economy has always been an important engineering consideration in any process industry. A successful process design will permit greater economy in yielding products. Optimization in turn plays a very important role in process design. In the study of the step aeration process, the distribution of the organic load and the flow behavior are found to be important variables which affect the optimal design of the process. In this study, four types of systems are investigated for the overall pattern of flow, mixing, and distribution of feed for the step aeration process. The combination of the discrete version of the maximum principle and the steepest descent search technique is used to carry out the optimization work.

CHAPTER II

MATHEMATICAL ANALYSIS OF THE PROCESS

1. PRINCIPLE OF AERATION AND KINETIC MODEL

(a) Principle of Biological Oxidation (6)

Biological oxidation is simply a conversion process therein dissolved organic compounds are converted into bacterial cells, which can then be removed from the waste water. The generalized reaction for the removal of soluble organics may be considered as follows:

$$\text{Organics} + O_2 + \text{Nutrients} \xrightarrow{\text{Organisms}} CO_2 + H_2O + \text{Organisms.}$$

(b) Growth Pattern (2)

The curve in Figure 5 illustrates the classic growth pattern exhibited by microorganisms in a batch culture. Examination of the curve reveals that growth passes through three different phases. Initially, all nutrients are present in excess of the requirements of the microorganism, and growth is unrestricted. During this period, called the constant growth phase, the concentration of microorganisms increases at an exponential rate. At some concentration, one of the nutrients becomes growth limiting and the culture proceeds into the declining growth phase. In response to the increasing competition of the microorganisms for the

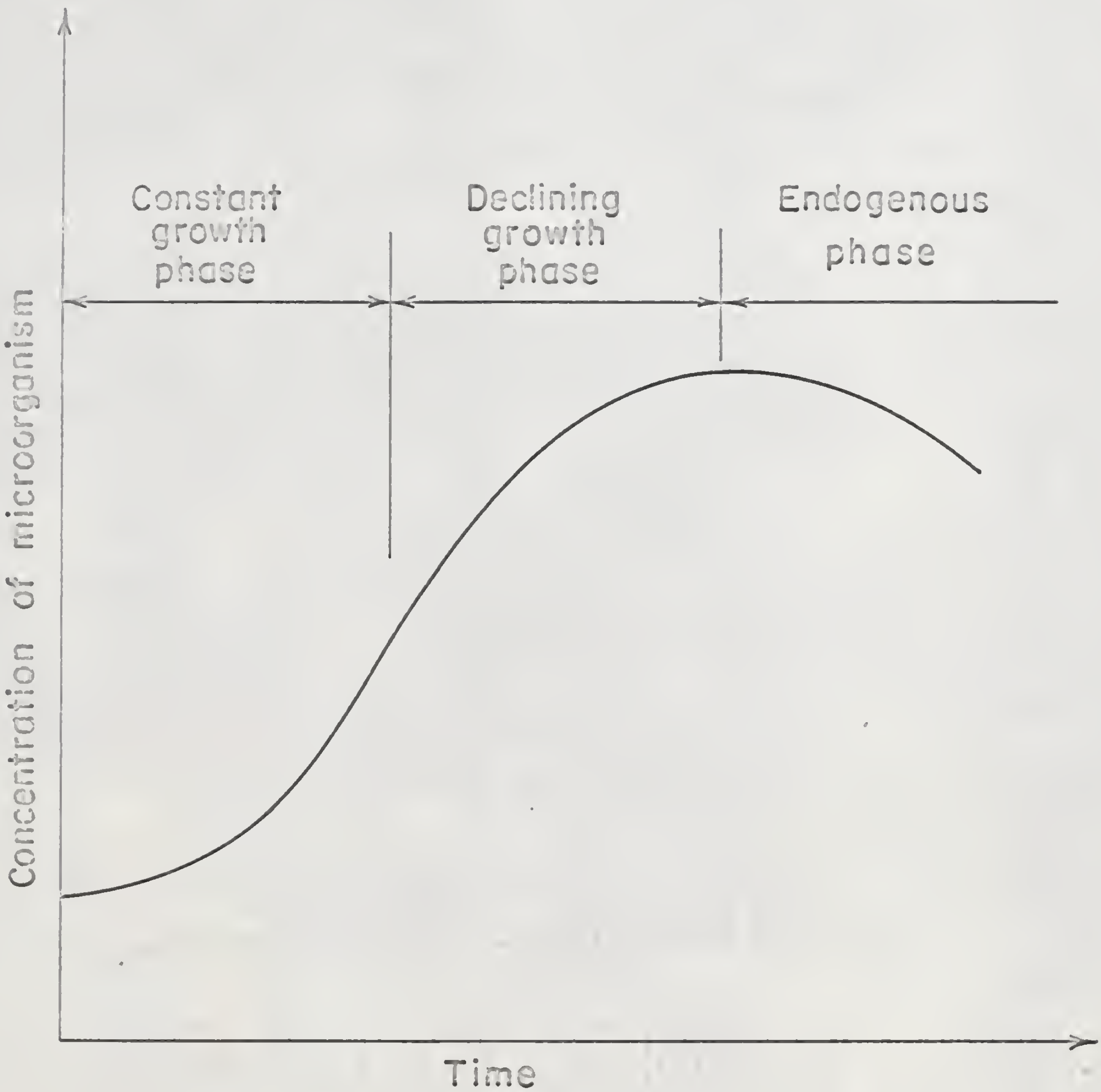


Fig. 5. Classic growth pattern.

remaining limiting nutrient, the rate of growth decreases until growth finally halts. The remaining portion of the curve represents the decrease of the microorganism resulting from autooxidation which occurs after the depletion of the available organics. This is often called the endogeneous respiration phase of activated sludge.

(c) Kinetic Model

As stated previously, in an aerobic environment not limited by mixing or nutrients, the specific growth rate is proportional to the concentration of organisms. The mathematical model, therefore, can be represented by

$$r = \frac{dx_4}{dt} = kx_4 \qquad (1)$$

where

r = growth rate, mg/liter, hr.,

x_4 = concentration of organisms, mg/liter,

k = growth rate constant, hr^{-1}.

Monod (7), in his study of bacterial growth in a chemostat (continuous culture), found that his data behaved in a manner typified by the Michaelis-Menten equation which is one of the most widely accepted models of enzyme kinetics. He therefore suggested the following form for the growth rate constant.

$$k = k^{s}_{max} \left(\frac{x_2}{K + x_2} \right) \tag{2}$$

where

k^{s}_{max} = maximum growth rate when the organic concentration is not limiting the rate of growth, hr^{-1},

K = the concentration of organics at which the specific growth rate observed is one half the maximum value; saturation constant, mg/liter,

x_2 = concentration of organics, mg/liter.

Then, if one milligram of organics produces Y milligrams of organisms, the rate of consumption of organics will be

$$r_s = \frac{dx_2}{dt} = - \frac{1}{Y} \frac{dx_4}{dt} . \tag{3}$$

From an engineering viewpoint, we may consider the various phases of sludge growth and BOD removal to consist of a dynamic relationship between the mass transfer of essential foods into the cell structure, and the assimilation and utilization of these foods for energy and growth. At high concentrations of organic matter, the rate of assimilation and the growth rate are independent of the concentration of organic matter. At low organic levels, the rate of growth and hence the rate of BOD removal are frequently concentration dependent. The kinetic form of Equation (2) describes the situation except during the endogenous phase.

Growth under the first phase is independent of the concentration of organics, x_2, since the organics are in excess i.e. $x_2 >> K$, and thus Equation (2) becomes

$$k = k^s_{max} .$$

During the initial part of the second phase of growth, k is dependent on x_2 and the original form of Equation (2) applies, but as the organics are consumed, x_2 becomes very small, i.e. $x_2 << K$ and Equation (2) simplifies to

$$k = \frac{k^s_{max} x_2}{K} . \qquad (4)$$

During the endogeneous phase, the effect of endogeneous respiration becomes important. In the expression for one phase kinetics proposed by Grieves et al. (8), the effect of endogeneous respiration is considered. The expression is

$$r = \frac{k^s_{max} x_2}{K+x_2} x_4 - k^D x_4 \qquad (5)$$

where

k^D = the specific endogeneous microbial attrition rate, hr^{-1}.

when $x_2 >> K$, Equation (5) becomes

$$r = k^s_{max} x_4 - k^D x_4 = (k^s_{max} - k^D) x_4 , \qquad (6)$$

and when $x_2 << K$, Equation (5) becomes

$$r = \frac{k_{max}^{s} \; x_2 x_4}{K} - k^D x_4. \tag{7}$$

Theoretically, when

$$x_2 = \frac{k^D K}{k_{max}^{s}}$$

we have

$$r = 0.$$

Numerically k^D is usually two orders of magnitude less than k_{max}^{s}. Hence the effect of endogeneous respiration is negligible except when x_2 is very small. Therefore, the model represented by Equation (2) is used in the present work.

2. THE MATHEMATICAL REPRESENTATION OF THE PROCESS

(a) Flow Models

A plug flow model is often used to represent the flow behavior of the conventional activated sludge process. This model assumes that there is no longitudinal mixing in the aeration tank. However, the optimum degree of longitudinal mixing in the aeration tank is still in question. Some investigator (9) has advocated the use of aeration tanks designed to provide a uniform composition within the entire tank. The latter system is often referred to as the complete mixing activated sludge process (9) and the completely mixed stirred tank model is usually used to represent the flow behavior in this system.

In step aeration, the influent is fed to the reactor system at several different points in order to avoid the confinement of growth and oxidation to one end of the basin as in the conventional process. Furthermore, from the kinetic model we can see that feeding a larger amount of feed to the front end will increase the organic concentration but dilute the organism concentration. Therefore, a step aeration process with appropriate distribution of organic load may perform better than the conventional process. A series of plug flow units in which feed enters at the inlet of each plug flow unit can be used to represent the flow behavior of the process. Similarly, the step aeration process can also be represented by a sequence of continuously stirred tanks in which feed enters the system at several points.

(b) Simplifying Assumptions

The following assumptions and simplifications are made in specifying the process and developing the mathematical representation for the process.

(1) The system is isothermal and is under the steady state condition.

(2) Physical properties such as density, diffusivity, and viscosity are constant.

(3) Y is dependent only upon the property of the waste itself, and independent of the age of the organisms and the effect of other physical conditions such as the concentrations of organics and organisms.

(4) Organics and organisms are distinctly separate entities in solution.

(5) Endogeneous respiration does not influence the system performance.

(6) The sludge and waste streams are completely mixed at each point where the waste is introduced.

(7) Sufficient oxygen is supplied for the oxidation.

(8) The fluid is a continuum and there is no segregation.

Some of these assumptions depart from reality. They are justified on the grounds that they simplify the relationship of the process without appreciably changing the basic characteristics of itself.

(c) The Mathematical Representation

Based on the preceding assumptions and the flow models described in the previous section we can visualize the system as consisting of mixing stages and reaction stages as shown in Figure 6. For convenience, we consider these

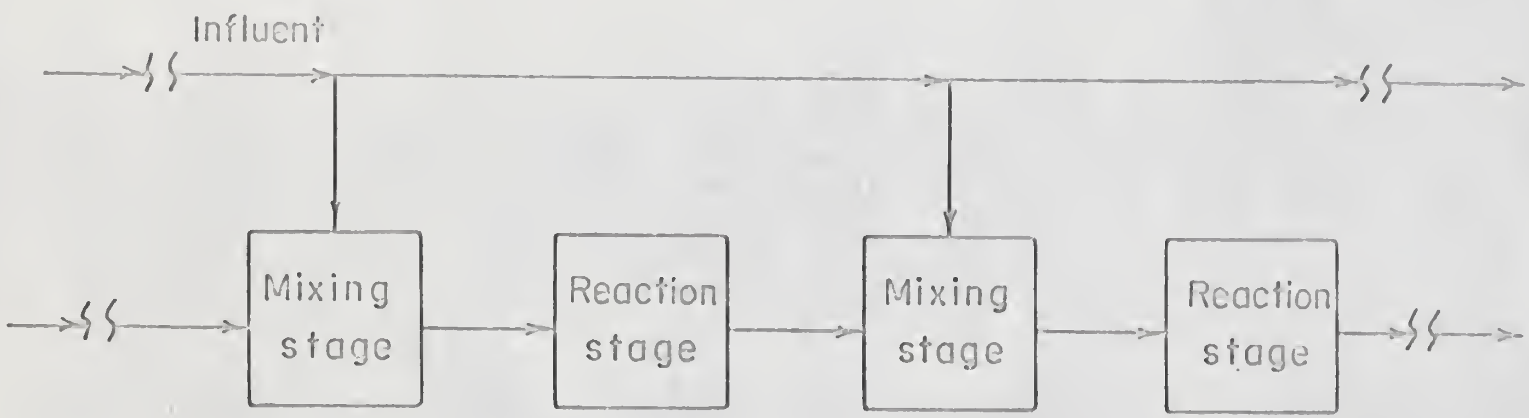


Fig. 6 Model of step aeration activated sludge process.

two different parts separately and number each stage as shown in Figure 7. We also define the following notations for the subsequent analysis.

x_1^{2n} = volumetric rate of the flow discharged from the 2n th stage, liter/hr,

x_2^{2n} = concentration of organics in the outlet stream of the 2n th stage, mg/liter,

x_2^f = concentration of organics in feed, mg/liter,

x_3^{2n} = accumulated volume up to and including the 2n th stage, liters,

x_4^{2n} = concentration of organisms in the outlet stream of the 2n th stage, mg/liter,

x_4^f = concentration of organisms in feed, mg/liter,

θ_1^{2n-1} = volumetric rate of waste introduced at the (2n-1)th stage, liter/hr,

θ_2^{2n} = volume of the 2n th stage, liters.

(1) Analysis of a mixing stage

In order to establish a mathematical model of the mixing stage, we visualize the (2n-1)th stage as shown in Figure 8(a), and the essential governing equations are written

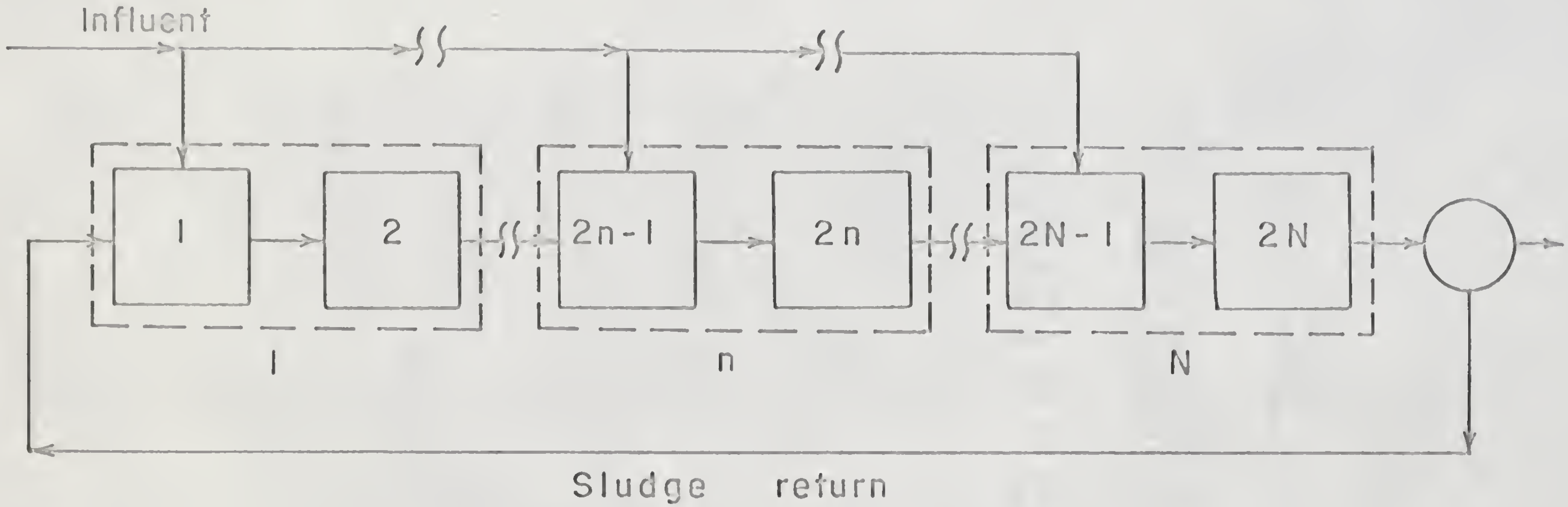
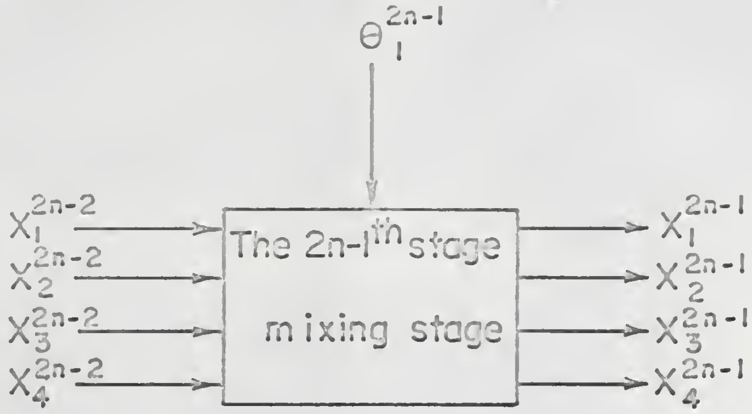
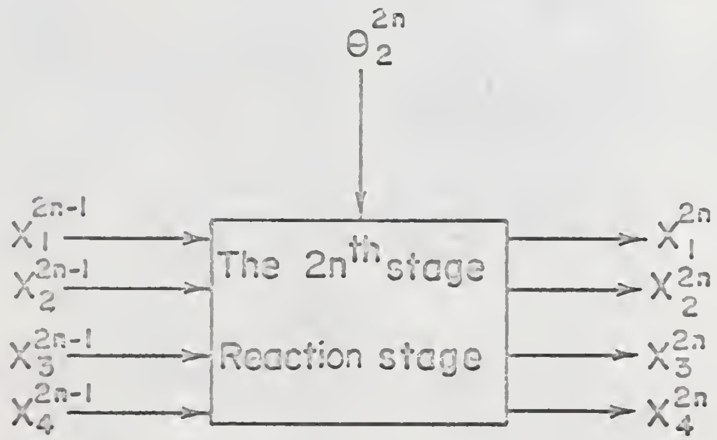


Fig. 7. N reactor model of step aeration activated sludge process.



(a) Mixing stage



(b) Reaction stage

Fig.8 A schematic representation of a mixing stage and a reaction stage.

based on the assumed kinetic and flow models using the notations established above.

i. overall material balance.

$$x_1^{2n-1} = \theta_1^{2n-1} + x_1^{2n-2} . \qquad (8)$$

ii. material balance of the oxidizable organics.

$$\theta_1^{2n-1} x_2^f + x_2^{2n-2} x_1^{2n-2} = x_2^{2n-1} x_1^{2n-1} . \qquad (9)$$

Using Equations (8) and (9) to eliminate x_1^{2n-1} and solving for the exit concentration of organics, x_2^{2n-1}, we obtain

$$x_2^{2n-1} = \frac{\theta_1^{2n-1} x_2^f + x_2^{2n-2} x_1^{2n-2}}{\theta_1^{2n-1} + x_1^{2n-2}} \qquad (10)$$

iii. organism material balance.

$$\theta_1^{2n-1} x_4^f + x_4^{2n-2} x_1^{2n-2} = x_4^{2n-1} x_1^{2n-1} . \qquad (11)$$

Since x_4^f is assumed to be equal to zero and, as given by Equation (8),

$$x_1^{2n-1} = \theta_1^{2n-1} + x_1^{2n-2},$$

Equation (11) becomes

$$x_4^{2n-1} = \frac{x_1^{2n-2}\ x_4^{2n-2}}{\theta_1^{2n-1} + x_1^{2n-2}} . \tag{12}$$

iv. accumulated volume.

$$x_3^{2n-1} = x_3^{2n-2}. \tag{13}$$

The mixing stage is assumed to mix without capacity.

(2) Analysis of a reaction stage

A reactor stage designated as the 2n th stage is shown in Figure 8(b). The essential governing equations are derived below.

i. overall material balance.

$$x_1^{2n} = x_1^{2n-1} . \tag{14}$$

ii. organism material balance. The quantity of organisms produced in each reactor can be expressed in terms of the quantity of organics consumed, that is,

$$x_1^{2n}\ x_4^{2n} - x_1^{2n-1}\ x_4^{2n-1} = Y(x_1^{2n-1}\ x_2^{2n-1} - x_1^{2n}\ x_2^{2n}), \tag{15}$$

where Y denotes the yield factor of the biochemical oxidation process. Using Equation (14), Equation (15) can be simplified to

$$x_4^{2n} - x_4^{2n-1} = Y(x_2^{2n-1} - x_2^{2n}) \ . \tag{16}$$

iii. accumulated volume.

$$x_3^{2n} = x_3^{2n-1} + \theta_2^{2n} \ . \tag{17}$$

iv. organic material balance. The rate of growth is determined by the concentration of organisms and organics at each point within the reactor, which is in turn influenced by the flow model used. Therefore, the complete mixing model and the plug flow model yield two different material balances for the oxidizable organics.

Since the exit stream from the continuous flow stirred tank reactor has the same concentration of organics and organisms as the fluid within the reactor, Equations (1), (2) and (3) can be combined to give, if the completely stirred tank system is considered,

$$-r_s = \frac{kx_4^{2n}}{Y} = \frac{k_{max}^{s}}{Y} \left(\frac{x_2^{2n}}{K + x_2^{2n}}\right) x_4^{2n} \ . \tag{18}$$

The corresponding organic material balance is

$$x_1^{2n-1}\ x_2^{2n-1} - x_1^{2n}\ \ x_2^{2n} + r_s\, \theta_2^{2n} = 0 \ . \tag{19}$$

If we substitute Equation (18) into Equation (19), the organic material balance becomes

$$x_1^{2n-1}\ x_2^{2n-1} - x_1^{2n}\ \ x_2^{2n} - \frac{k_{max}^s\ x_2^{2n}\ \ x_4^{2n}\ \theta_2^{2n}}{Y(K + x_2^{2n}} = 0 \qquad (20)$$

For this system, the concentration of organisms, x_4^i, is dependent upon that of organics, hence x_4^i can be expressed as function of x_2^i. By applying the initial stage up to and including the ith stage, we obtain

$$x_4^i = \frac{1}{x_1^i}\ \ x_1^0\ x_4^0 + Yx_1^0\ x_2^0 + Yx_1^i\ x_2^f - Yx_1^0\ x_2^f - Yx_1^i\ x_2^i$$

$$= \frac{A_o}{x_1^i} + Yx_2^f - Yx_2^i\ , \quad i = 1, 2, \ldots 2N, \qquad (21)$$

where

$$A_o = x_1^0\ x_4^0 + Yx_1^0\ x_2^0 - Yx_1^0\ x_2^f \qquad (22)$$

Since the plug flow model assumes that there is no mixing of fluid longitudinally along the flow path, the concentration of organics and organisms varies from position to position along the reactor. Therefore, the material balance for organics must be made for a differential element of volume dV.

Referring to Figure 9, the material balance is

$$x_1^{(2n)}(\ell)\ x_2^{(2n)}(\ell) - x_1^{(2n)}\ (\ell + d\ell)\ \ x_2^{(2n)}(\ell + d\ell) + r_s^{(2n)} A\ d\ell$$

$$= 0 \qquad (23)$$

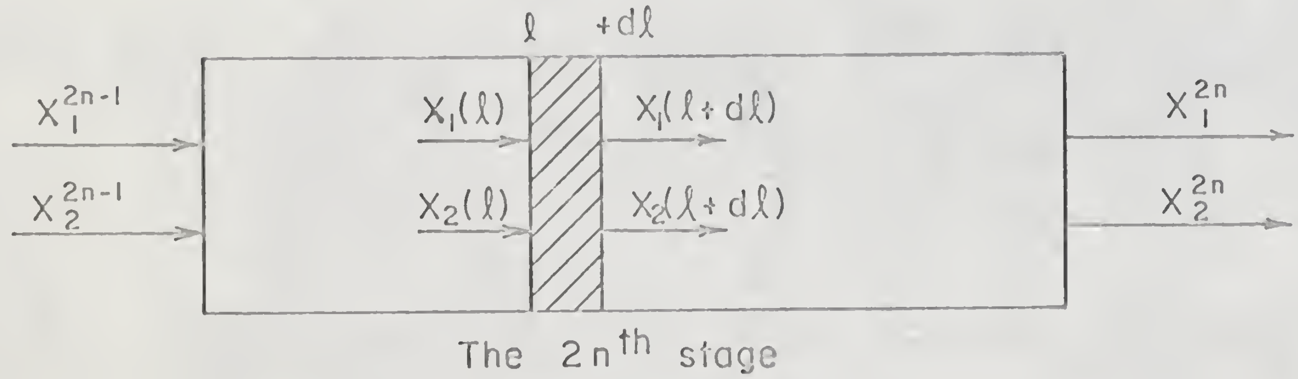


Fig. 9. Differential element of a plug flow reactor.

where $x_1^{(2n)}(\ell)$ and $x_1^{(2n)}(\ell + d\ell)$ are the volumetric flow rates at positions ℓ and $\ell + d\ell$ respectively of the 2n th stage, $x_2^{(2n)}(\ell)$ and $x_2^{(2n)}(\ell + d\ell)$ are the concentration of organics at positions ℓ and $\ell + d\ell$ respectively of the 2n th stage, and $r_s^{(2n)}$ is the reaction rate within the differential volume, dV, between ℓ and $\ell + d\ell$. Since density is constant, the volumetric flow rateis unchanged along the plug flow reactor. Therefore, Equation (23) can be simplified and becomes

$$-x_1^{(2n)}(\ell)\, dx_2^{(2n)}(\ell) + r_s^{(2n)} A\, d\ell = 0 \, . \tag{24}$$

Rearranging this equation gives

$$\frac{dx_2^{(2n)}(\ell)}{d\ell} = \frac{A}{x_1^{(2n)}(\ell)}\, r_s^{(2n)} \, , \tag{25}$$

where

$$r_s^{(2n)} = \frac{-k\overline{x_4^{(2n)}}(\ell)}{Y} = \frac{-k_{max}^{s}\, x_2^{(2n)}(\ell)\, x_4^{(2n)}(\ell)}{Y\left[K + x_2^{(2n)}(\ell)\right]} \, . \tag{26}$$

where $x_4^{(2n)}(\ell)$ is the concentration of organisms at the position ℓ of the 2n th stage, which is dependent upon $x_2^{(2n)}(\ell)$. Since $x_1^{(2n)}(\ell)$ is constant throughout the stage, Equation (25) can be integrated if $x_4^{(2n)}(\ell)$ can be expressed in terms of $x_2^{(2n)}(\ell)$.

Referring to Figure 10, the overall organism material balance from the 1st stage up to the position ℓ of the 2n th stage can be used to express $x_4^{(2n)}(\ell)$ as

$$x_4^{(2n)}(\ell) = a - Yx_2^{(2n)}(\ell), \tag{27}$$

where

$$a = \frac{1}{x_1^{2n-1}} \left[x_1^0 x_4^0 + Yx_1^0 x_2^0 - Yx_1^0 x_2^f \right] . \tag{28}$$

If we substitute Equation (27) into Equation (25) and integrate by applying the boundary conditions,

$$x_2^{(2n)}(0) = x_2^{2n-1} \quad \text{and} \quad x_2^{(2n)}(L) = x_2^{2n} \tag{29}$$

we obtian

$$AL = \theta_2^{2n} = -\left[\frac{K}{ac} + \frac{1}{Yc}\right] \ell n \frac{(a - Yx_2^{2n-1})}{(a - Yx_2^{2n}} - \frac{K}{ac} \ell n \left(\frac{x_2^{2n}}{x_2^{2n-1}}\right). \tag{30}$$

where θ_2^{2n} is the reactor volume of the 2n th stage.

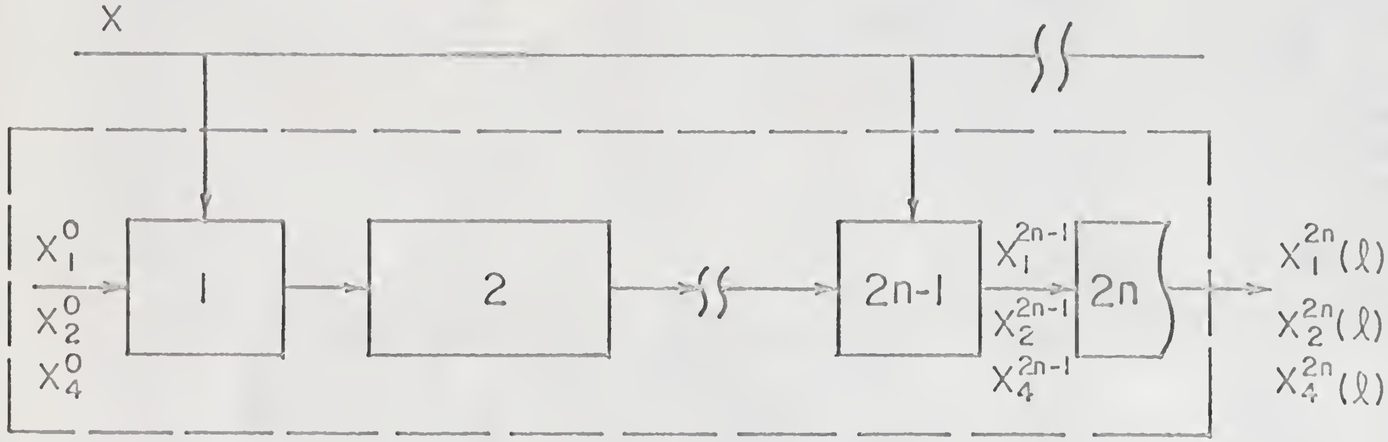


Fig. 10. Schematic representation of plug flow reactors in series system

CHAPTER III

SYSTEM ANALYSIS AND SIMULATION

1. SYSTEM ANALYSIS

An analysis of the system to determine the number of independent variables or degrees of freedom is often required for designing and optimizing comples systems. In this analysis, an N stage system is considered; however, each stage is assumed to consist of a mixing stage and a reaction stage; thus, the actual model we consider is composed of 2N stages. (see Figures 7 and 8)

(1) Type and Number of System Variables

a) Volumetric flow rate of feed,

θ_1^{2n-1}, $\quad n = 1,1 \ldots N; \quad N$

b) Volumetric flow rate through each stage,

x_1^i, $\quad i = 0, 1, \ldots 2N; \quad 2N + 1$

c) Organic concentrations,

x_2^i, $\quad i = 0, 1, \ldots 2N; \quad 2N + 1$

d) Organism concentrations,

x_4^i, $\quad i = 0, 1, \ldots 2N; \quad 2N + 1$

e) Reactor volume at each stage,

θ_2^{2n}, $n = 1, \ldots N;$ N

f) Concentrations of organics and organisms in feed,

x_2^f and x_4^f; 2

$\therefore$ Total number of system variables = $3(2N + 1)$

$+ 2N + 2 = 8N + 3.$

(2) Type and Number of Relations Among System Variables,

a) Material balance of organic component,

(i) Mixing stages,

$$x_1^{2n-2}\ x_2^{2n-2} + \theta_1^{2n-1}\ x_2^f = x_1^{2n-1}\ x_2^{2n-1}, \quad n = 1, \ldots N; \quad N$$

(ii) Reaction stages (Tank reactor is under consideration),

$$x_1^{2n-1}\ x_2^{2n-1} + r_s\ \theta_2^{2n} = x_1^{2n}\ x_2^{2n}, \quad n = 1, \ldots N; \quad N$$

b) Material balance of organism component.

(i) Mixing stages,

$$x_1^{2n-2}\ x_4^{2n-2} + \theta_1^{2n-1}\ x_4^f = x_1^{2n-1}\ x_4^{2n-1}, \quad n = 1, \ldots, N; \quad N$$

(ii) Reaction stages,

$$x_4^{2n} - x_4^{2n-1} = Y(x_2^{2n-1} - x_2^{2n}), \quad n = 1, \ldots, N; \quad N$$

c) Overall material balance at each stage.

(i) Mixing stages,

$$x_1^{2n-2} + {}_1^{2n-1} = x_1^{2n-1}, \quad n = 1, \ldots, N; \quad N$$

(ii) Reaction stages,

$$x_1^{2n-1} = x_1^{2n-2}, \quad n = 1, \ldots, N; \quad N$$

d) Total number of relations = 6N.

(3) Degree of Freedom of System.

From the total number of variables and relations obtained in previous sections, the number of degrees of freedom for the entire system is

$$F = 8N + 5 - 6N = 2N + 5 .$$

If the system is specified by the variables, x_1^0, x_2^0, x_4^0, x_1^{2N}, x_2^{2N}, x_2^f, x_4^f, then the number of degrees of freedom becomes

$$F = 2N + 5 - 7 = 2N - 2 .$$

2. SIMULATION STUDY

In order to obtain a better understanding of the behavior of the system represented by the proposed model, a simulation study has been carried out. Because it is difficult to represent graphically a system with a high number of dimensions, only a two-stage completely mixed flow reactor system has been considered.

The N stage system is schematically shown in Figures 6 and 7. When N = 2, this diagram corresponds to the two-stage completely mixed flow system used in this simulation study. In accordance with the derivation in the previous section, two degrees of freedom exist in this problem (i.e. $F = 2 \cdot 2 - 2 = 2$). The amount of the allocation of waste water in the first stage, θ_1^1, and the reactor volume of the first stage, θ_2^2, are chosen as being the two decision variables for this study.

By using the material balance equations, Equation (2.8) through (2.20), as derived in the previous chapter, and the assigned boundary conditions, x_1^0, x_2^0, x_4^0, x_1^4, x_2^4, x_2^f, x_4^f, and the two specified decision variables, θ_1^1, θ_2^2, the overall accumulated reactor volume, x_3^4, can be evaluated. The simulation study has been carried out by systematically altering the values of θ_1^1 and θ_2^2 and computing the value of x_3^4 for each case.

The following data are employed: $Y = 0.5$, $k^s_{max} = 0.1$ hr^{-1}, $K = 100$ mg/ℓ, $x^f_2 = 800$ mg/ℓ, $x^f_4 = 0$ mg/ℓ, $x^0_1 = 1800$ ℓ/hr, $x^0_2 = 150$ mg/ℓ, $x^0_4 = 8000$ mg/ℓ, $x^4_1 = 6000$ ℓ/hr, $x^4_2 =$ 80 mg/ℓ.

Numerical computation for this simulation has been performed with an IBM computer 1620 and the numerical results are listed in Table 1.

Figure 11 shows a plot of the allocation of sewage in the first stage versus the overall accumulated volume with the volume of the first stage as parameter. From this figure a two-dimensional surface level diagram is in turn plotted in Figure 12.

From Figures 11 and 12 it can be seen that the objective function for minimizing the overall reactor volume is a unimodal function. The minimum point is located at the position where 3900 liters per hour of sewage feed are introduced into the first stage and where the reactor volume of the first stage is 6250 liters.

In Figure 12 are also plotted two searching loci obtained by the discrete version of the maximum principle with the steepest descent search technique as discussed in a later chapter. The one stage system can be obtained as a special case in this simulation study by assigning no reactor volume and no allocation of sewage feed in the first stage. For this special case of one completely mised reactor system, a reactor volume of 14,833 liters is required to obtain the

Table 1. Overall Reactor Volume Computed in the Simulation of a System Composed of Two Completely Stirred Tanks in Series, liters.

$\bar{E}\,(\frac{\cdot}{hr})$ / σ_2^2 (l.)	3200	3400	3600	3800	4000	4200	4400
5500	11259	11171	11139	11155	11212	11301	11414
5750	11310	11194	11135	11128	11166	11239	11341
6000	11378	11233	11148	11117	11134	11190	11279
6250	11460	11289	11177	11122	11117	11155	11228
6500	11557	11359	11222	11142	11114	11133	11190
6750	11666	11444	11281	11176	11126	11124	11163
7000	11787	11541	11354	11225	11151	11128	11149
7250	11918	11650	11439	11286	11189	11144	11147
7500	12059	11770	11536	11360	11240	11174	11156

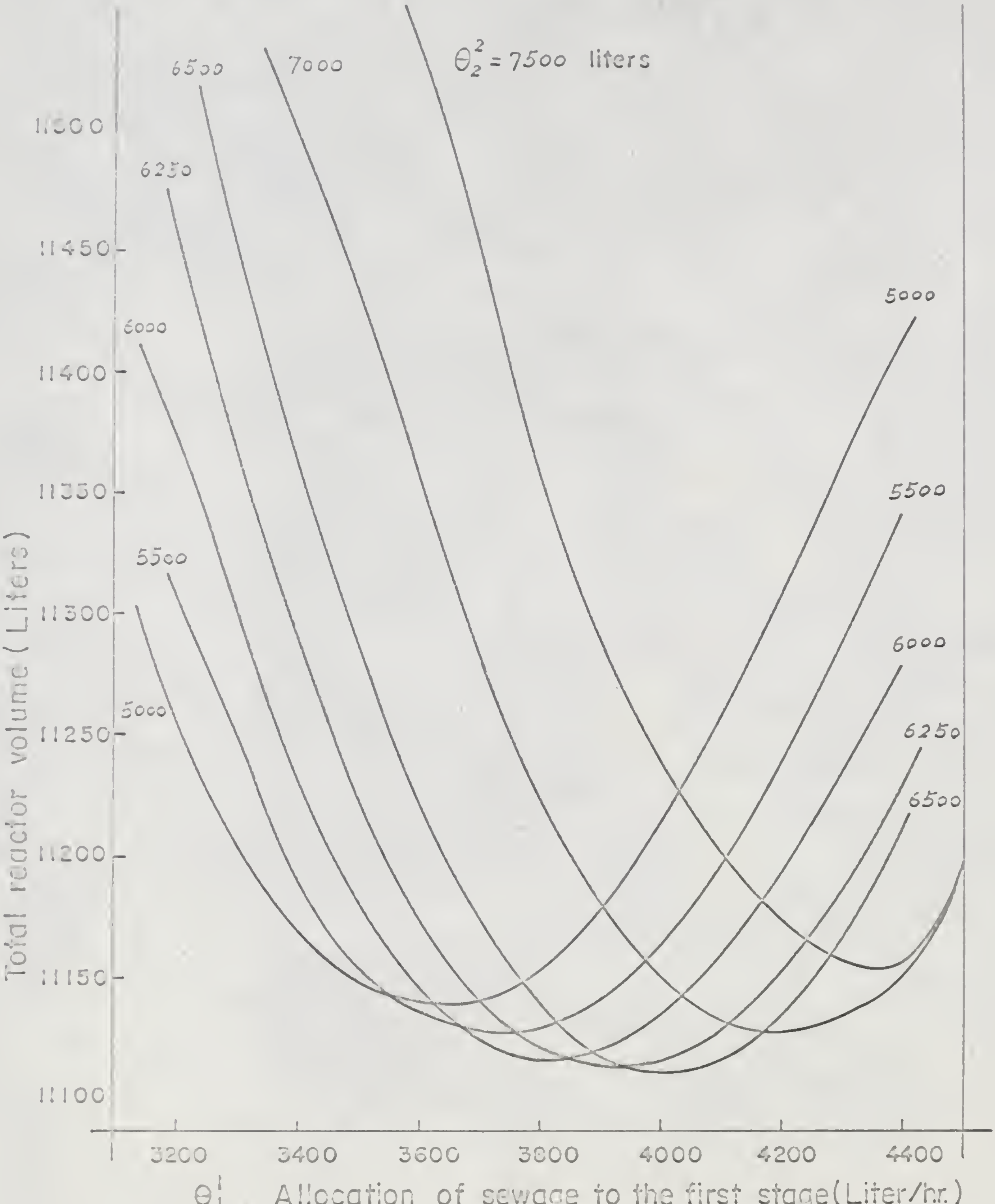


Fig. 11. Overall accumulated volume vs. allocation of sewage to the first reactor with the volume of the first reactor as parameter.

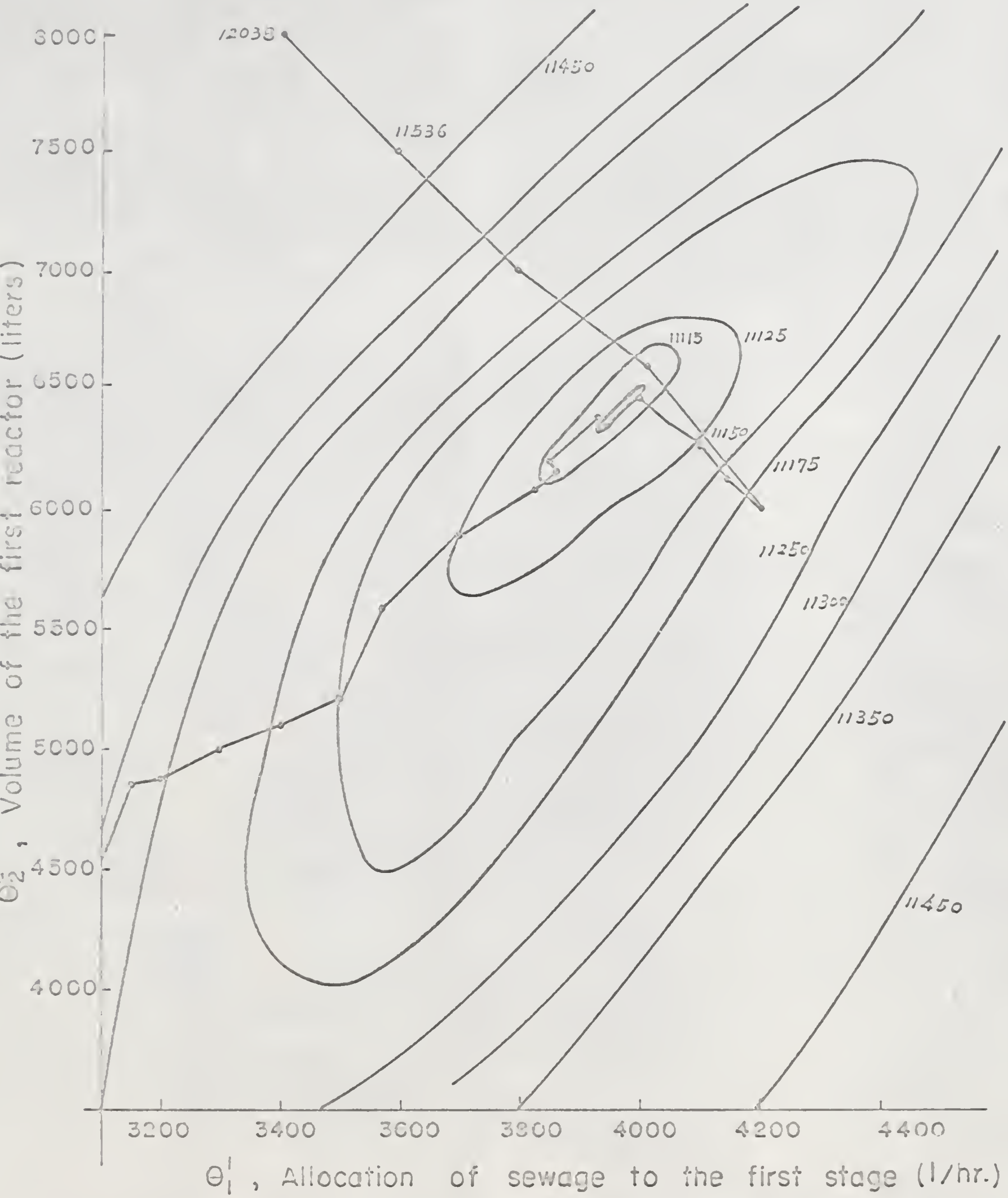


Fig. 12. Surface contours for the system and the searching locuses.

desired amount of the waste treatment. According to the analysis in the previous section, there is no optimization problem for this system since no degree of freedom exists.

CHAPTER IV

OPTIMIZATION STUDY OF THE PROCESS

In the previous chapter, the simulation study has been performed for the two-stage complete mixing system. When a more complicated system is being treated, it becomes very time consuming to use simulation to optimize the system. There are a number of techniques that can be used to optimize complicated systems. Some of these include (A) differentiation, (B) linear and nonlinear programming, (C) dynamic programming, (D) experimental search techniques, and (E) the maximum principle. The descrete maximum principle is a powerful technique for treating multistage sequential systems, and it will be used to optimize several models of the system we are considering. However, before treating the multistage step aeration systems a brief description of the discrete maximum principle will be given.

1. THE DISCRETE MAXIMUM PRINCIPLE (10)

(1) Statement of The Algorithm for Simple Processes.

A schematical representation of a simple sequential stagewise process is shown in Figure 13. The state of the process stream denoted by an s-dimensional vector, $x = (x_1, x_2, \ldots, x_s)$, is transformed at each stage according to the decisions, denoted by a t-dimensional vector, $\theta = (\theta_1, \theta_2, \ldots, \theta_t)$, made at that stage. The transformation

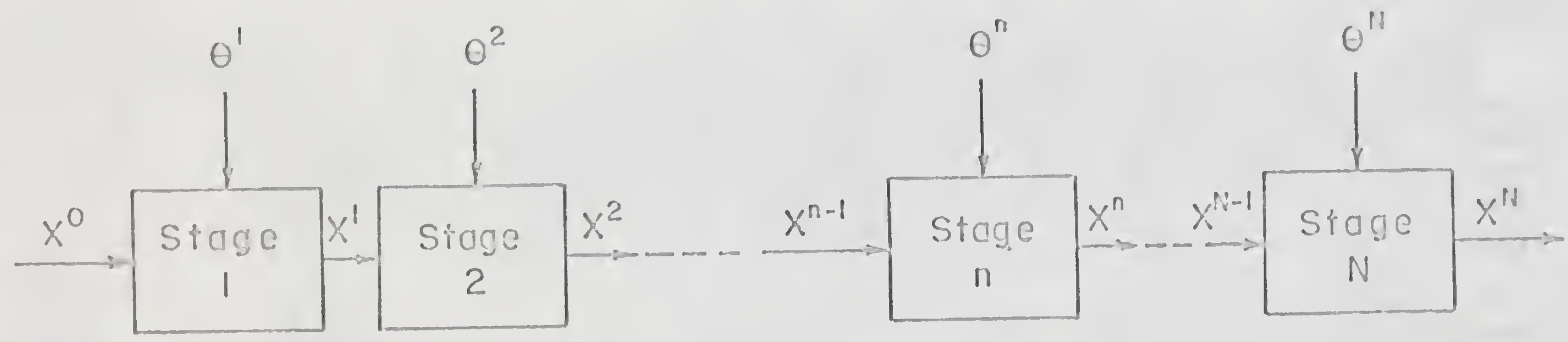


Fig. 13. Simple sequential multistage process. x represents the state vector ; θ represents the decision vector.

of the process stream at the nth stage is described by a set of performance equations represented by

$$x_i^n = T_i^n \, (x_1^{n-1}, x_2^{n-1}, \ldots, x_s^{n-1}, \theta_1^n, \theta_2^n, \ldots \theta_t^n), \; i = 1, 2, \ldots s \qquad (1)$$

where T_i^n is a transformation operator for component i at the nth stage. The optimization problem which we want to consider here is one in which all the initial conditions, x_1^0, x_2^0, ..., x_s^0, are given, and one of the end conditions, x_k^N, is preassigned. For this optimization problem, we assume the objective function is of the form,

$$S = \sum_{\substack{i=1 \\ i \neq k}}^{s} c_i x_i^N \; . \qquad (2)$$

The problem we wish to consider is one in which we want to extremize this objective function subject to these given initial and end conditions, and the equality conditions given by Equation (1).

The algorithm for solving such an optimization problem by the discrete maximum principle is to introduce an s-dimensional adjoint vector, z^n, and a Hamiltonian function H^n satisfying

$$H^n = \sum_{i=1}^{s} z_i^n \, T_i^n \, (x^{n-1}; \theta^n), \quad n = 1, 2, \ldots, N \qquad (3)$$

$$z_i^{n-1} = \frac{\partial H^n}{\partial x_i^{n-1}} \qquad i = 1, 2, \ldots s \qquad n = 1, 2, \ldots N. \tag{4}$$

and

$$z_i^N = c_i \qquad i = 1, 2, \ldots s \qquad i \neq k\ . \tag{5}$$

The optimal sequence of decisions θ_i^n is determined from the condition,

$$\frac{\partial H^n}{\partial \theta_i^n} = 0\ ; \qquad i = 1, 2, \ldots t \qquad n = 1, 2, \ldots N, \tag{6}$$

when the decision variables lie in the interior of the domain of the decision variables. If the optimal decision variables lie on the boundary of the domain, then the Hamiltonian function, H^n, should be an extremum at the boundary. Both x and z are considered as fixed in extremizing the Hamiltonian.

(2) Computational Scheme.

The analytical and numerical solutions will be outlined for a process in which one end stage state variable x_k^N is fixed.

a) Analytical solution. Referring to Figure 13, all initial conditions x_i^o are given, and x_k^N is also fixed (where i = 1, ..., s). Now we are to find the numerical values for the following variables at the optimal conditions:

$$
\begin{array}{ll}
{}_{i}^{n}, & i = 1, 2, \ldots, t \\
 & n = 1, 2, \ldots, N, \\
x_i^n, & i = 1, 2, \ldots, s \\
 & n = 1, 2, \ldots, N \\
 & \text{except } x_k^N, \\
z_i^n, & i = 1, 2, \ldots, s \\
 & n = 1, 2, \ldots, N, \\
s &
\end{array}
$$

The total number of unknowns as established above are

$$t \cdot N + 2 \cdot s \cdot N + 1 - 1 = t \cdot N + 2 \cdot s \cdot N.$$

The available relations are summarized as follows:

Relation	Number of relations
1. Performance relations, Equation (1)	$s \cdot N$
2. $z_i^N = c_i$, $i \neq k$, Equation (5)	$s-1$
3. Adjoint relations, Equation (4)	$s \cdot (N-1)$
4. $\dfrac{\partial H^n}{\partial \theta_i^n} = 0$, Equation (6)	$t \cdot N$
5. Objective function Equation (2)	1

The total number of relations is, therefore,

$$s \cdot N + s \cdot (N-1) + (s-1) + (t \cdot N) + 1 = t \cdot N + 2 \cdot s \cdot N.$$

Since the number of variables is equal to the number of relations, the desired quantities can be found by solving the equations simultaneously. The simultaneous solution of these equations is extremely difficult except for some simple cases. Because of this, numerical procedures for treating the particular type of problems under consideration have been developed (10).

b) Numerical solution

The numerical computation for the process can be carried out by the following steps.

Step 1. Assume a set of values for θ_i^n ($i = 1, 2, \ldots, t$; $n = 1, 2, \ldots, N$) except for θ_k^N. Since x_k^N is given, θ_k^N will be a dependent variable.

Step 2. Calculate all the state variables x_i^n ($n = 1, 2, \ldots, N-1$; $i = 1, 2, \ldots, s$) by using the corresponding performance equations.

Step 3. Calculate θ_k^N from the performance equation,

$$x_k^N = T_k^N (x^{N-1}, \theta^N).$$

Step 4. Calculate x_i^N ($i = 1, 2, \ldots, k-1, k+1, \ldots, s$) from the corresponding performance equation, i.e.,

$$x_i^N = T_i^N (x^{N-1}, \theta^N) \; ; \; i = 1, 2, \ldots, k-1, k+1, \ldots, s,$$

with the θ_k^N value obtained from step 3.

Step 5. Calculate all

$$\frac{\partial x_i^n}{\partial x_j^{n-1}} \text{ and } \frac{\partial x_i^n}{\partial \theta_\ell^n}$$

with all state variables and decision variables obtained from previous steps.

In a multistage operation with one end stage state variable, say x_k^N, fixed, the adjoint variable associated with it, namely z_k^N, should be dependently determined to hold

$$\frac{\partial H^N}{\partial \theta_k^N} = \sum_{i=1}^{s} z_i^N \frac{\partial x_i^N}{\partial \theta_k^N} = 0 \; , \tag{8}$$

we thus obtain

$$z_k^N = \frac{-\sum\limits_{\substack{i=1 \\ i \neq k}}^{s} z_i^N \dfrac{\partial x_i^N}{\partial \theta_k^N}}{\dfrac{\partial x_k^N}{\partial \theta_k^N}} \; . \tag{9}$$

Step 6. Using Equation (5) and the corresponding derivatives obtained from Step 5, z_k^N can be calculated from Equation (9).

Step 7. Calculate the remaining adjoint variables, i.e., z_i^n ($n = 1, 2, \ldots, N - 1$; $i = 1, 2, \ldots, s$) from Equation (4).

Step 8. Calculate all values of $\frac{\partial H^n}{\partial \theta_i^n}$ ($n = 1, 2, \ldots, N$; $i = 1, 2, \ldots, t$) except $\frac{\partial H^n}{\partial \theta_k^N}$ from Equation (6).

If the values of θ_i^n are not the optimal values, the values of $\frac{\partial H^n}{\partial \theta_i^n}$ ($n = 1, 2, \ldots, N$; $i = 1, 2, \ldots, t$) will not be zero. We define

$$\frac{\partial H^n}{\partial \theta_i^n} = \phi_i^n \,(z^n, x^{n-1}, \theta^n).$$

Step 9. Using the method of steepest descent a new set of decisions can be found to replace the old set according to the following equations

$$(\theta_i^n)_{new} = (\theta_i^n)_{old} + \Delta \theta_i^n, \quad \begin{array}{l} i = 1, 2, \ldots, t \\ n = 1, 2, \ldots, N \end{array} \tag{10}$$

where $\Delta \theta_i^n$, $i = 1, 2, \ldots, t$; $n = 1, 2, \ldots, N$ are specified small correcting values whose sign is determined by that of the corresponding ϕ_i^n.

Step 10. If all the values of ϕ_i^n ($n = 1, 2, \ldots N$; $i = 1, 2, \ldots t$) are smaller than some preassigned small values ε_i, then the set of θ_i^n is approximately the optimal decision set and the iteration should be stopped. If not, the computation goes back to step 1.

2. OPTIMIZATION STUDIES OF STEP AERATION SYSTEM CONSISTING OF SEVERAL COMPLETELY-STIRRED REACTORS IN SERIES

As mentioned in Chapter 1, the distribution of the organic load and the flow behavior are important variables in the step aeration process which affect the optimal design of a process. In this section the effect of these variables on the volume required for a specified degree of treatment will be considered for the step aeration process composed of several completely-stirred tanks in series.

The problem is to determine the distribution of the organic load which minimizes the total required reactor volume for such a system. In Chapter 2, this system is described in detail and the related system equations are derived (see Figures 6, 7, and 8).

(1) Formulation of the Problem

The problem is to find the optimal allocation of the sewage and the optimal distribution of volumes between allocations for carrying out the waste treatment process in a sequence of completely stirred tank reactors so that the total reactor volume is minimized. The objective function of this problem is therefore simply represented as

$$S = x_3^{2N} \tag{11}$$

where x_3^{2N} represents the total reactor volume.

The related performance equations have been derived previously. As shown in Figures 6, 7 and 8 the odd numbered stages account for the mixing process which is described mathematically as follows:

From Equation (2.8), the overall material balance is

$$x_1^{2n-1} = \theta_1^{2n-1} + x_1^{2n-2} \ . \tag{12}$$

From Equation (2.10), the material balance of the oxidizable organics is

$$x^{2n-1} = \frac{\theta_1^{2n-1} \ x_2^{f} + x_2^{2n-2} \ x_1^{2n-2}}{\theta_1^{2n-1} + x_1^{2n-2}} \tag{13}$$

From Equation (2.13), the accumulated volume is

$$x_3^{2n-1} = x_3^{2n-2} \ . \tag{14}$$

The even numbered stages account for the biological growth process which is described mathematically as follows: From Equation (2.14), the overall material balance leads to

$$x_1^{2n} = x_1^{2n-1} \ . \tag{15}$$

From Equations (2.20) and (2.21), the material balance of the oxidizable organics gives

$$x_1^{2n-1} x_2^{2n-1} - x_1^{2n-1} x_2^{2n} - \theta_2^{2n} \frac{k_{max}^s}{Y} \frac{x_2^{2n}\left(\frac{A_o}{x_1^{2n-1}} + Yx_2^f - Yx_2^{2n}\right)}{K + x_2^{2n}}$$

$$= 0 . \tag{16}$$

Equation (16) can be generally expressed as

$$x_2^{2n} = f\ (x_1^{2n-1}, x_2^{2n-1}, \theta_2^{2n}). \tag{17}$$

From Equation (2.19), the accumulated volume is

$$x_3^{2n} = x_3^{2n-1} + \theta_2^{2n} . \tag{18}$$

In applying a discrete form of the maximum principle to determine the optimal policy for the system as stated above, the following Hamiltonian functions and adjoint variables are introduced. The Hamiltonian functions for the mixing stages and reaction stages, respectively, are

$$H^{2n-1} = \sum_{i=1}^{3} z_i^{2n-1} x_i^{2n-1}, \quad n = 1, 2, \ldots, N, \tag{19}$$

$$H^{2n} = \sum_{i=1}^{3} z_i^{2n} x_i^{2n}, \quad n = 1, 2, \ldots, N . \tag{20}$$

The adjoint variables for the mixing and reaction stages, respectively, are

$$\lambda_j^{2n-2} = \frac{\partial f^{2n-1}}{\partial x_j^{2n-2}} - \sum_{i=1}^{3} \lambda_i^{2n-1} \frac{\partial x_i^{2n-1}}{\partial x_j^{2n-2}}, \quad j = 1, 2, 3, \quad n = 1, 2, \ldots N, \tag{21}$$

$$\lambda_j^{2n-1} = \frac{\partial f^{2n}}{\partial x_j^{2n-1}} - \sum_{i=1}^{3} \lambda_i^{2n} \frac{\partial x_i^{2n}}{\partial x_j^{2n-1}}, \quad j = 1, 2, 3, \quad n = 1, 2, \ldots N. \tag{22}$$

Differentiating Equations (12), (13), and (14) with respect to x_j^{2n-2} for $j = 1, 2, 3$, and substituting the results into Equation (21) gives, for $j = 1, 2$, and 3, respectively

$$\lambda_1^{2n-2} = \lambda_1^{2n-1} + \lambda_2^{2n-1} \frac{(u_1^{2n-1} + x_1^{2n-2})x_2^{2n-2} - (u_1^{2n-1}x_2^{f} + x_1^{2n-2}x_2^{2n-2})}{(u_1^{2n-1} + x_1^{2n-2})^2}, \tag{23}$$

$$\lambda_2^{2n-2} = \lambda_2^{2n-1} \frac{x_1^{2n-2}}{(u_1^{2n-1} + x_1^{2n-2})} \tag{24}$$

$$\lambda_3^{2n-2} = \lambda_3^{2n-1}, \tag{25}$$

Similarly, differentiating Equations (15), (16), and (17) with respect to x_j^{2n-1} for $j = 1, 2, 3$, and substituting the results into Equation (22) gives, for $j = 1, 2$, and 3, respectively

$$z_1^{2n-1} = z_1^{2n} + \frac{1}{B} \left\{ (K + x_2^{2n})(x_2^{2n-1} - x_2^{2n}) \right.$$

$$\left. + \theta_2^{2n} x_2^{2n} \frac{k_{max}^s}{Y} \frac{A_o}{(x_1^{2n-1})^2} \right\}, \tag{26}$$

$$z_2^{2n-1} = z_2^{2n} \frac{x_1^{2n-1}}{B} (K + x_2^{2n}), \tag{27}$$

$$z_3^{2n-1} = z_3^{2n}, \tag{28}$$

where

$$B = Kx_1^{2n-1} + 2x_1^{2n-1} x_2^{2n} - \theta_2^{2n} k_{max}^s x_2^{2n} - x_1^{2n-1} x_2^{2n-1}$$

$$+ \theta_2^{2n} \frac{k_{max}^s}{Y} \left(\frac{A_o}{x_1^{2n-1}} + Y x_2^f - Y x_2^{2n}\right).$$

Since x_1^{2N} and x_2^{2N} are specified, the only boundary condition for the adjoint variables in this system is

$$z_3^{2N} = 1. \tag{29}$$

From Equations (25), (28), and (29), we thus obtain

$$z_3^{2n-1} = z_3^{2n} = 1, \quad n = 1, 2, \ldots, N. \tag{30}$$

According to the so-called weak form of the discrete maximum principle, the optimal decision variables at each stage must satisfy the equations

$$\frac{\partial H^{2n-1}}{\partial \theta_1^{2n-1}} = \sum_{i=1}^{3} z_i^{2n-1} \frac{\partial x_i^{2n-1}}{\partial \theta_1^{2n-1}} = 0 \,, \quad n = 1, 2, \ldots, N, \tag{31}$$

and

$$\frac{\partial H^{2n}}{\partial \theta_2^{2n}} = \sum_{i=1}^{3} z_i^{2n} \frac{\partial x_i^{2n}}{\partial \theta_2^{2n}} = 0 \,, \quad n = 1, 2, \ldots, N. \tag{32}$$

If the optimal decision variables are in the interior of the domain by differentiating Equations (12), (13), and (14) with respect to θ_1^{2n-1}, Equation (31) becomes

$$\frac{\partial H^{2n-1}}{\partial \theta_1^{2n-1}} = z_1^{2n-1} + z_2^{2n-1}$$

$$\frac{(\theta_1^{2n-1} + x_1^{2n-2})x_2^f - (\theta_1^{2n-1}x_2^f + x_2^{2n-2}\ x_1^{2n-1})}{(\theta_1^{2n-1} + x_1^{2n-2})^2} = 0,$$

$$n = 1, 2, \ldots, N \,. \tag{33}$$

By differentiating Equations (15), (16), and (18) with respect to θ_2^{2n} and substituting the resulting expressions into Equation (32) it becomes

$$\frac{\partial H^{2n}}{\partial \theta_2^{2n}} = - z_2^{2n} \frac{x_2^{2n}}{B} \frac{k^s_{max}}{Y} \left(\frac{A_o}{x_1^{2n-1}} + Y x_2^f - Y x_2^{2n}\right) + 1 = 0 ,$$

$$n = 1, 2, \ldots, N. \qquad (34)$$

If the optimal decision variables are on the boundary of the domain, the corresponding value of H^{2n-1} or H^{2n} must be an extremum.

(2) Computational Scheme

Numerical solutions to the system of algebraic equations given by Equations (12), (13), (14), (15), (16), (18), (23), (24), (26), (27), (30), (33), and (34) are obtained by following the computational scheme presented previously. For this problem, the step by step computational procedure is as follows:

Step 1. Assume values for θ_1^{2n-1}, θ_2^{2n}, $n = 1, 2, \ldots, N-1$.

Step 2. Using the given conditions, i.e., x_1^0, x_2^0, x_3^0, x_1^{2N}, x_2^{2N}, calculate the state variables, x_i^{2n-1}, and x_i^{2n}, $i = 1, 2, 3$, $n = 1, 2, \ldots, N$, and ${}_1^{2N-1}$, ${}_2^{2N}$ from Equations (12) through (18).

Step 3. Using Equation (34) for $n = N$, calculate z_2^{2N}.

Step 4. Using Equation (27) for $n = N$, calculate z_2^{2N-1}.

Step 5. Using Equation (33) for $n = N$, calculate z_1^{2N-1}.

Step 6. Then using Equations (23), (24), (26), and (27), calculate the rest of the adjoint variables z_1^{2n-1}, z_2^{2n-1}, z_1^{2n} and z_2^{2n}, $n = 1, 2, \ldots, N-1$.

Step 7. Calculate the values of $\dfrac{\partial H^{2n-1}}{\partial \theta_1^{2n-1}}$ and $\dfrac{\partial H^{2n}}{\partial \theta_2^{2n}}$ from Equations (33) and (34), which are represented by ϕ_1^{2n-1} and ϕ_2^{2n} respectively. (Note: If the values of θ_1^{2n-1} and θ_2^{2n} are not the optimal values, the values of ϕ_1^{2n-1} and ϕ_2^{2n} will not be zero).

Step 8. Using the following equations, calculate the new set of decision variables.

$$(\theta_1^{2n-1})_{new} = (\theta_1^{2n-1})_{old} + (\Delta\theta_1^{2n-1})(\mathrm{sgn}\,\phi_1^{2n-1}),$$

$$(\theta_1^{2n})_{new} = (\theta_1^{2n})_{old} + (\Delta\theta_2^{2n})(\mathrm{sgn}\,\phi_2^{2n}),$$

$$n = 1, 2, \ldots, N-1$$

where

$$\mathrm{sgn}\,\phi \begin{array}{l} = 1 \text{ if } \phi < 0 \\ = -1 \text{ if } \phi > 0. \end{array}$$

$\Delta\theta_1^{2n-1}$ and $\Delta\theta_2^{2n}$ are specified small constants.

Step 9. If all the values of ϕ_1^{2n-1} and ϕ_2^{2n} ($n = 1, 2, \ldots, N-1$) are smaller than some preassigned small values ϵ_i, then the set of θ_1^{2n-1} and θ_1^{2n} ($n = 1, 2, \ldots, N-1$) are approximately the optimal decision set and the iteration can be stopped. If not, the computation should go back to Step 1.

In the present work the numerical computation according to the above procedure has been performed with an IBM 1620 computer. The computer source program for a two-stage system is given in Appendix 1.

A slight modification of the above numerical procedure is required for those systems in which there is no allocation to one or more stages. The inequality constraint

$$\theta_1^{2n-1} \geqslant 0$$

must be satisfied at each stage; that is, the allocation to each tank must be either positive or zero. This inequality constraint is treated by setting θ_1^{2n-1} equal to zero for any stage in which a negative value for θ_1^{2n-1} is obtained in the numerical computation. For those stages with zero allocation, ϕ_1^{2n-1} should be positive and H^{2n-1} should be a minimum at the optimum. Thus, the zero value for θ_1^{2n-1} is maintained in the numerical computation as long as ϕ_1^{2n-1} is positive.

(5) Results and Discussion

Numerical results which give the optimal influent distribution and the optimal volume distribution for the step aeration system consisting of several completely stirred tanks in series are presented in this section. The kinetic constants are assigned the following values: $Y = 0.5$ mg/mg, $K = 100$ mg/liter, $k^s_{max} = 0.1$ hr^{-1}. The following additional conditions are also specified: $R = 0.4$, $x^0_2 = 150$ mg/ℓ, $x^0_3 = 8000$ mg/ℓ, $x^f_2 = 800$ mg/ℓ, $x^{2N}_2 = 80$ mg/ℓ, $\sum_{n=1}^{N} \theta^{2n-1}_1 = 4500$ ℓ/hr.

Numerical solutions have been obtained using these data for step aeration systems containing one, two, three, four, and five completely stirred tanks-in-series. The minimum volume, the optimal influent flow rates, and the optimal tank volumes are presented in Table 2 for each system. The relationship between the minimum volume of the system and the number of completely stirred tanks employed in the system is shown in Figure 14. The curve which is drawn through the set of discrete points shows that the total required aeration system volume decreases exponentially as the number of tanks in the system is increased. This is due to two important effects, the extent of longitudinal mixing in the aeration system and the method of feeding the influent to the system.

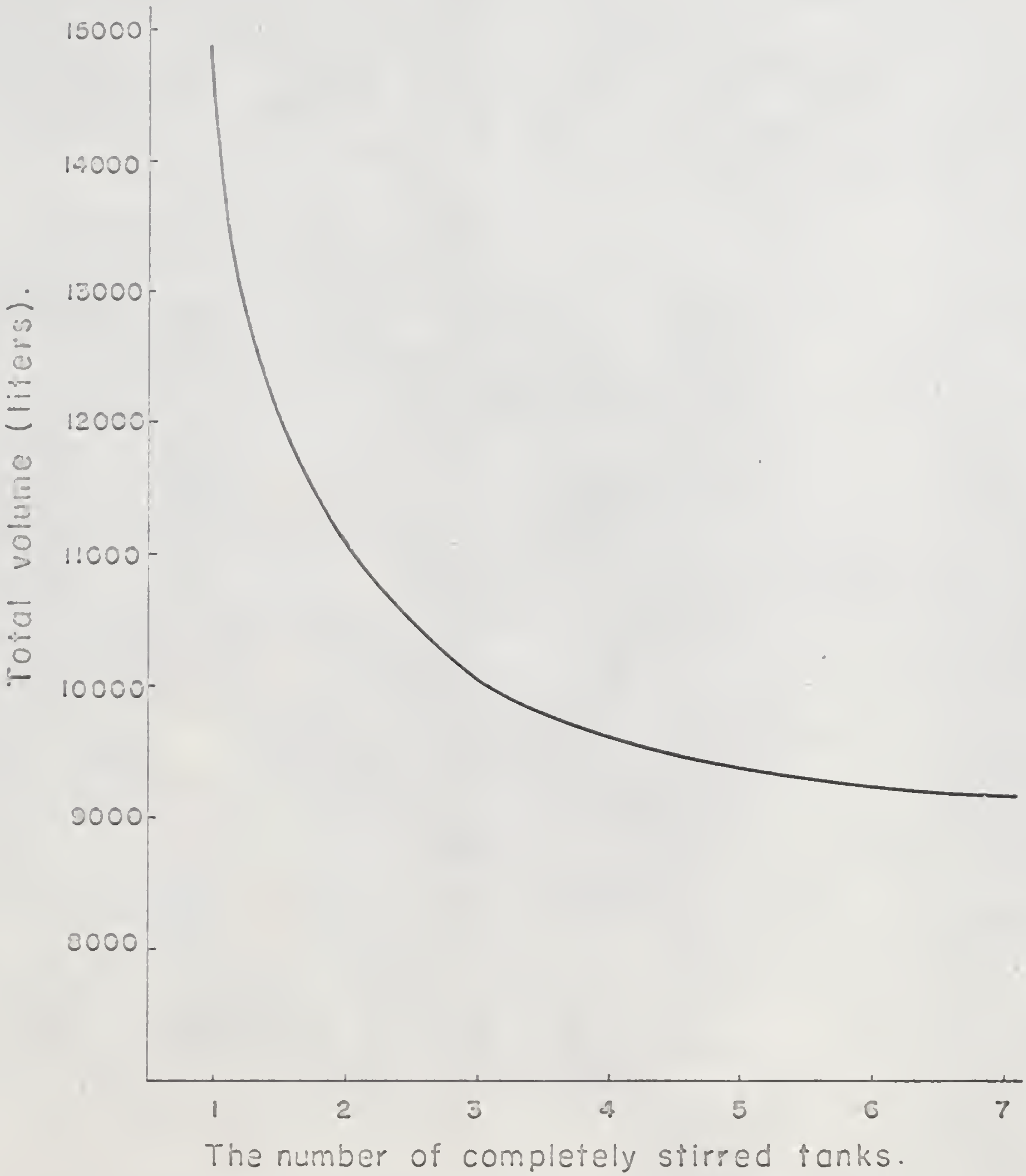


Fig. 14. Optimal total reactor volume v.s. the number of operating tanks for completely stirred tanks connected in series.

The amount of longitudinal mixing in the aeration system is related to the number of completely stirred tanks connected in series in the system. The one stage system represents a system with complete longitudinal mixing while the two, three, four, and five stage systems correspond to aeration systems with less longitudinal mixing. As the number of completely stirred tanks in the system increases the amount of longitudinal mixing decreases. Figure 14 shows that the required volume for the aeration system decreases as the number of tanks in the system increases. This indicates that as the amount of longitudinal mixing is decreased, the required volume decreases. The results for the three, four, and five stage systems in Table 2 show conclusively that longitudinal mixing is undesirable in the last part of the aeration system (the optimal volume of the last tank would be zero if longitudinal mixing were desirable). This result agrees with that of Bischoff (11) who has shown that longitudinal mixing is often undesirable in the last part of an aeration system.

The results in Table 2 also show that the optimal method of feeding the influent to the aeration system involves allocation of influent at more than one location. The Michaelis-Menten rate equation,

$$r = \frac{k^{c}_{max}\, x_2}{K + x_2}\, x_4 ,$$

Table 2. Optimal Operating Policies for a System Composed of a Sequence of Completely Stirred Tanks

Systems	Stage Number n	Optimal Policies: feed allocation, mg/ℓ. θ_1^{2n-1}	Optimal Policies: reactor volume, liters θ_2^{2n}	Optimal Total Volume, liters.
single stage	1	4500	14833	14833
two stages	1	3910	6260	
	2	590	4853	11113
three stages	1	3382	4103	
	2	1118	3598	
	3	0	2337	10038
four stages	1	3060	3400	
	2	1440	2779	
	3	0	2023	
	4	0	1419	9621
five stages	1	2820	3070	
	2	1660	2290	
	3	20	1690	
	4	0	1190	
	5	0	1162	9402

is used in this work to indicate that the growth rate depends on both the concentration of organics and organisms. We can see two counteracting effects that influence the growth rate when influent is added. The addition of influent increases the concentration of the organic substrate and decreases the concentration of the microorganisms. As shown in Table 2 the optimal method of feeding the five stage step aeration system involves distributing most of the influent to the first half of the system. In the first part of the system it is desirable to maintain as high a growth rate as possible by addint the influent in an optimal manner.

Influent should not be fed to the last part of the aeration system, because it is necessary to reduce the organic concentration to a specified small value at that end of the system. Near the exit, the addition of influent would increase the growth rate, but it would also greatly increase the organic concentration which has to be reduced to a specified value. As shown in Table 2, the optimal result is not to feed any influent to the last part of the aeration system.

The effect of the organism concentration, the organic concentration in the return sludge, and the return sludge flow rate on the optimal design have been studied for the aeration system containing two completely stirred tanks in series.

In Figure 15 and Table 3 are shown the optimal policies of the system for various inlet organism concentrations. The curve which relates the total optimal volume to the inlet organism concentration shows that an increase in the organism concentration in the return sludge will reduce the total required volume. This is due to the effect that an increase in organism concentration will favor the rate of growth. Curves which relate the optimal influent distribution and the optimal volume distribution to the inlet organism concentration are also shown in Figure 15. These results show that as the inlet organism concentration is increased a greater portion of the influent to the system should be fed to the second stage and a greater portion of the total volume should be allocated to that stage. Except for the organism concentration the data used in this study are the same as those given at the beginning of this section.

Similarly, the optimal policies for the two tank step aeration system with various inlet organic concentrations in the return sludge have been studied as shown in Figure 16 and Table 4. However, the data used in this part of the present study are slightly different, viz., $Y = 0.5$ mg/mg, $K = 100$ mg/l., $k^s_{max} = 0.13$ hr^{-1}, $R = 0.334$, $x^0_4 = 4000$ mg/l., $x^f_2 = 800$ mg/l. Figure 16 shows that the total optimal volume is nearly proportional to the organic concentration in the return sludge. The curves which relate the optimal influent

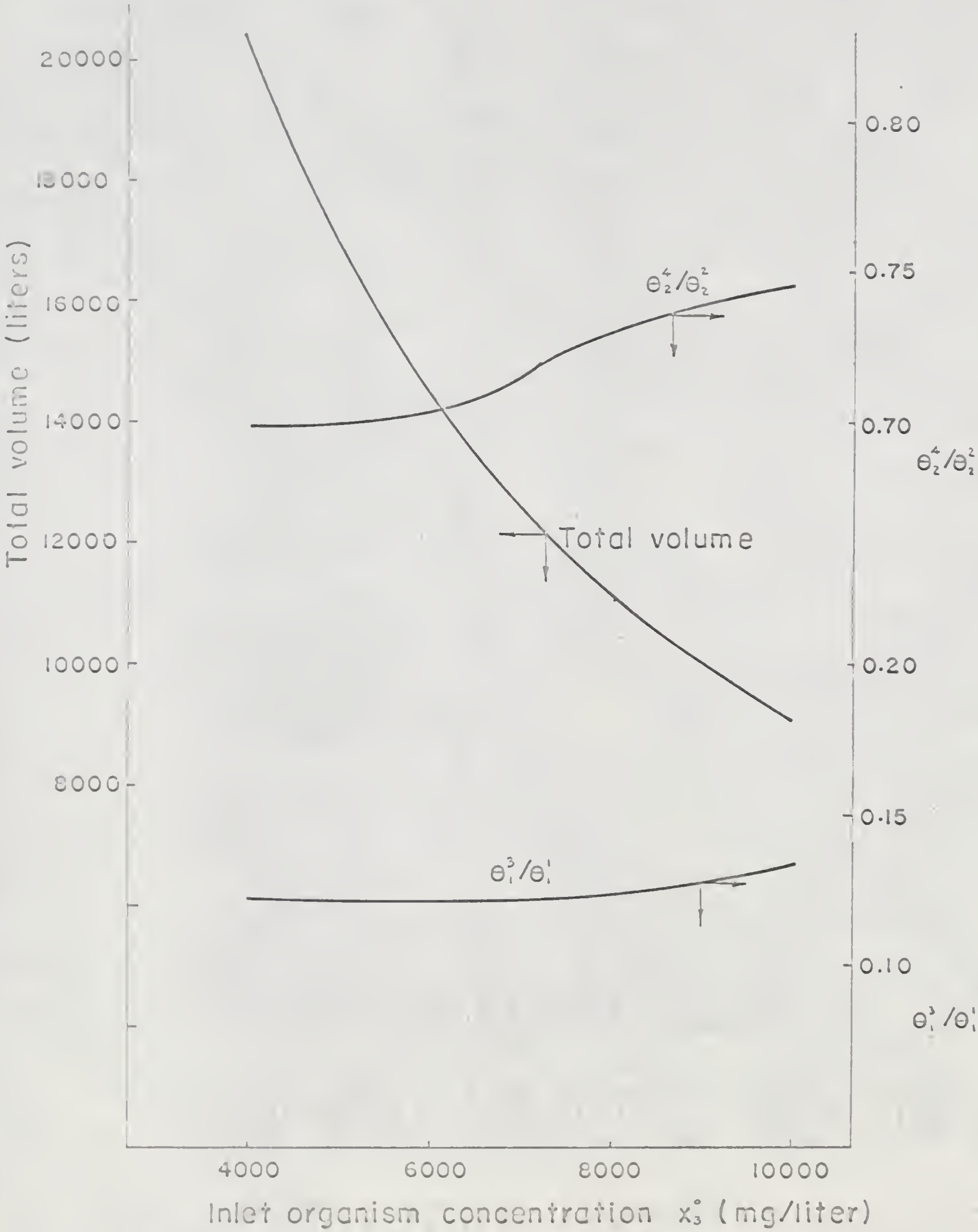


Fig. 15. Optimal total volume, feed distribution ratio, and volume distribution ratio as functions of the inlet organism concentration for the two tank step aeration system.

Table 3. Optimal Policies for a System Composed of Two [illegible] Stirred Tanks in Series for Various Inlet Organism Concentrations.

Inlet Organism Concentration, x_3^0 (mg./l.)	Optimal Feed Allocation (liters/hr) θ_1^1	θ_1^3	Optimal Volume Distribution (liters) θ_2^2	θ_2^4	Total Accumulated Volume (liters) x_3^4
4000	4010	490	12070	8382	20452
6000	4010	490	8475	5950	14425
8000	4000	500	6420	4693	11113
10,000	3970	530	5160	3858	9048

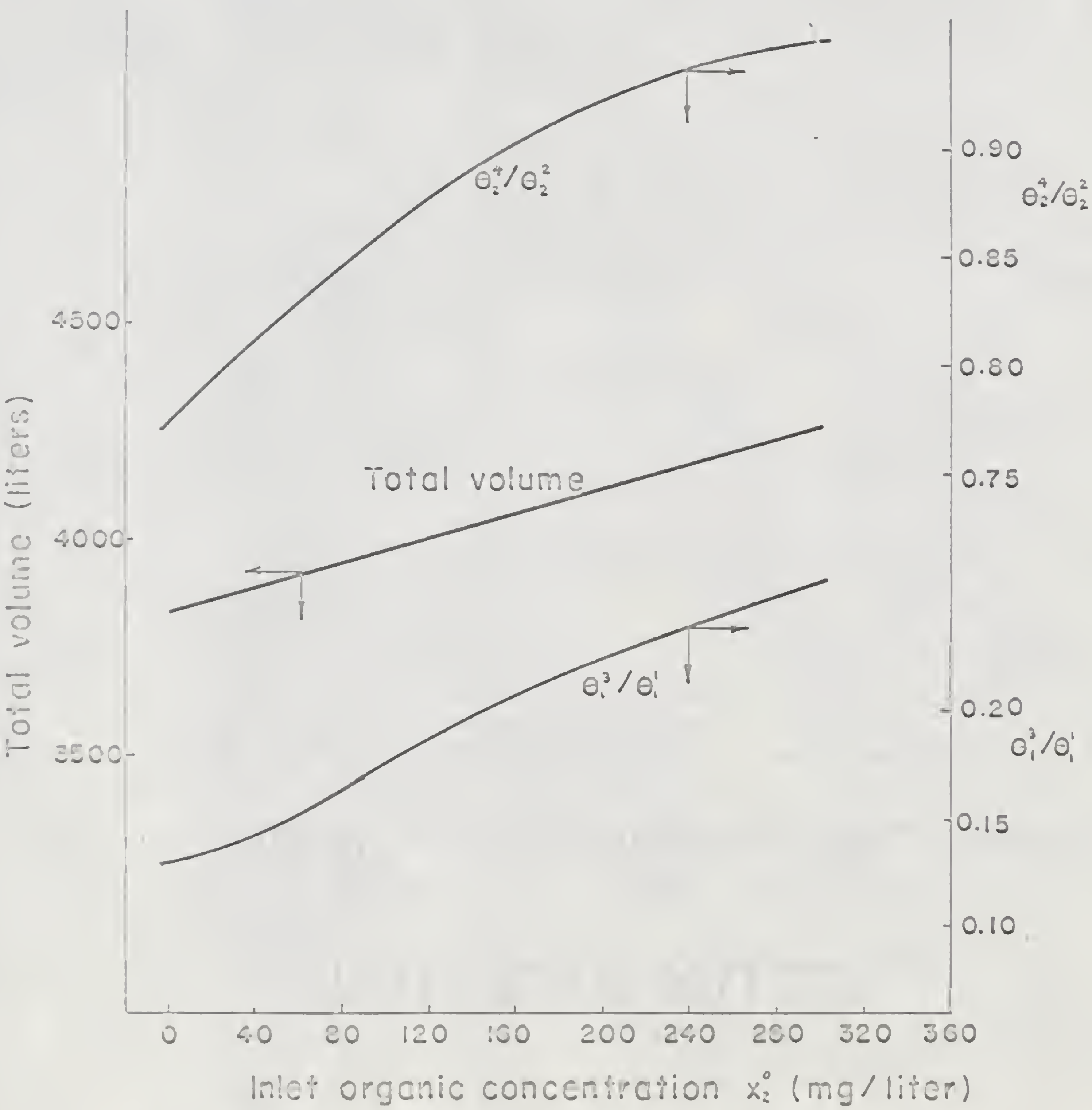


Fig. 16. Optimal total volume, feed distribution, and volume distribution ratio as functions of inlet organic for the two tank aeration system.

Table 4. Optimal Policies for a System Composed of Two Completely Stirred Tanks in Series for Various Inlet Organic Concentrations

Inlet Organic Concentration	Optimal Feed Allocation (liter/hr)		Optimal Volume Distribution (liters)		Total Accumulated Volume (liters)
x_2^0 (mg/ℓ)	Q_1^1	Q_1^3	Q_2^2	Q_2^4	x_3^4
0	3960	540	2140	1684.4	3824.4
40	3950	550	2150	1731.7	3881.7
80	3850	650	2140	1798.9	3938.9
150	3730	770	2130	1907.2	4037.2
300	3570	930	2170	2070.1	4240.1

distribution and the optimal volume distribution to the inlet organic concentration indicate that as the inlet organic concentration is increased a greater portion of the influent to the system should be fed to the second stage of the system and a greater portion cf the total volume should be allocated to that stage.

These results imply that an increase in either the organism or organic concentration in the return sludge will result in a smaller fraction of the influent and volume being allocated to the first stage. This effect appears to be due to an effort to take advantage of this increased inlet concentration in the first stage by reducing the amount of influent added to that stage.

Increasing the recycle ratio will reduce the volume required for the aeration system and thus reduce the capital cost associated with the volume requirements of the system. However, the costs associated with the sedimentation process and the cost of pumping the recycle stream will increase with an increase in the recycle flow rate. Furthermore, as more sludge is recycled through the system, the viscosity in the aeration system will increase and the cost of aeration will increase because of this. In order to show that there is an optimum recycle ratio, we assume a very simple cost model in which the total cost is given by

$$C_T = C_1 V + 4500\ C_2 R$$

where

C_1 = unit cost of volume, \$/liter

C_2 = unit cost of recycle ratio, \$-hr/liter

V = total volume, liters

R = recycle ratio, dimensionless.

In this expression each value of the total volume, V, is the optimal value determined by use of the maximum principle for a certain value of the recycle ratio, R. The optimal recycle ratio can be found graphically by plotting the total cost against the parameter, R.

The two stage model of the aeration system has been studied using this cost model for the case in which $C_1/C_2 = 0.5$.

In this study, the following data have been used. $Y = 0.5$ mg/mg, $K = 100$ mg/l, $k^s_{max} = 0.1\ hr^{-1}$, $x_2^0 = 150$ mg/l, $x_4^0 = 8000$ mg/l, $x_2^f = 800$ mg/l, $x_2^{2N} = 80$ mg/l, $\sum_{n=1}^{N} \theta_1^{2n-1} = 4500$ l/hr. The results which are presented in Table 5 and Figure 17 show that there is a minimum cost at R = 0.55.

Similarly, the optimal feed and volume distribution ratios are plotted in Figure 18. The curves show that the ratios decrease as the recycle ratio increases.

Table 5. Optimal Policies and Overall Costs for a System Composed of Two Completely Stirred Tanks in Series for Various Recycle Ratios.

Recycle Ratio	Optimal Feed Allocation (ℓ./hr)		Optimal Volume Distribution (liters)		Total Accumulated Volume (liters)	Overall Cost ($10,[illegible])
R	θ_1^1	θ_1^3	θ_2^2	θ_2^4	x_3^4	
0.2	3700	800	9060	7736	16796	9.398
0.4	3915	585	6245	4868	11113	7.357
0.6	4270	230	5520	3522	9042	7.222
0.9	4500	0	4845	2803	7648	7.674
1.5	4500	0	4080	2564	6644	10.072

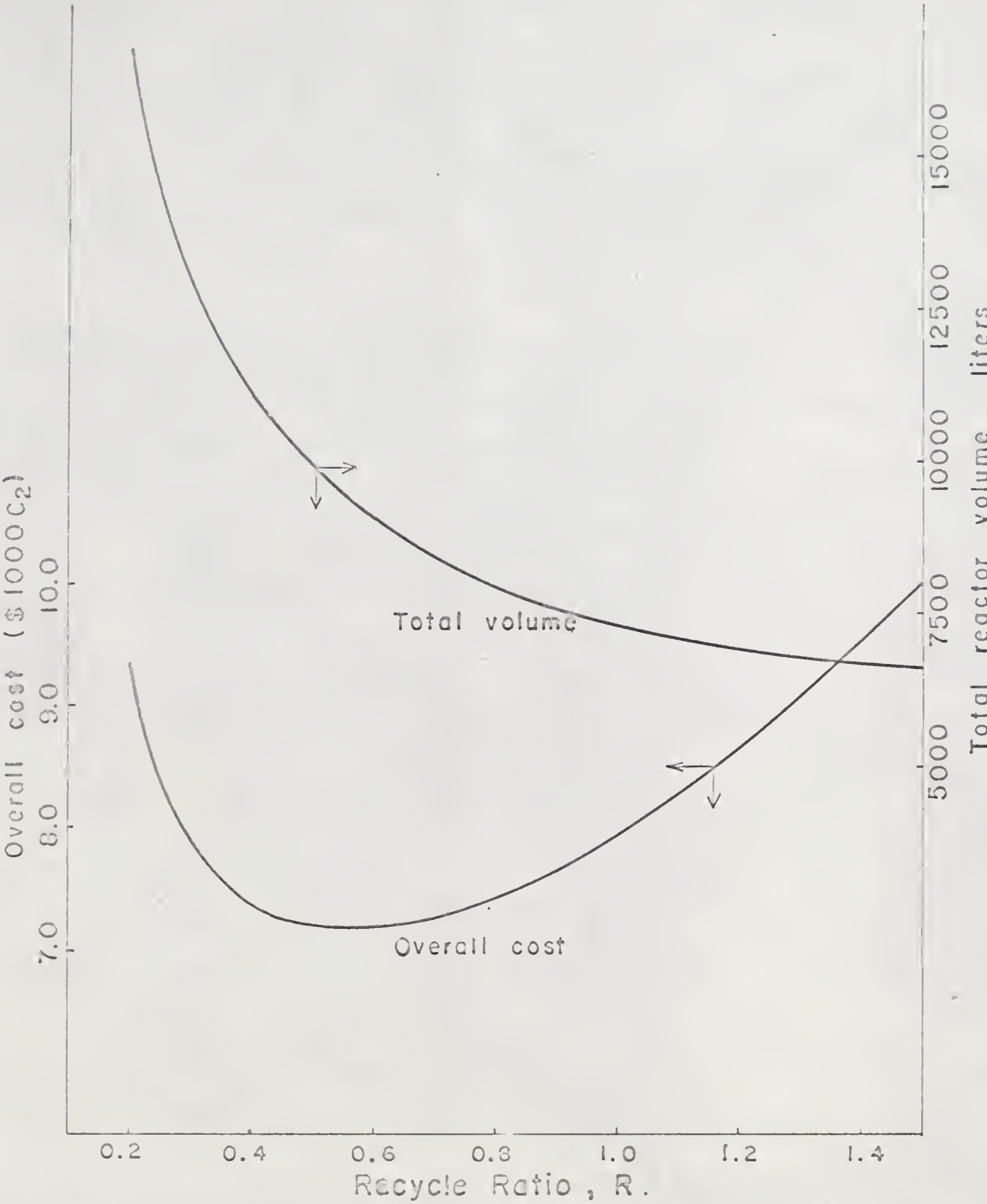


Fig.17. Overall cost and total volume v.s. recycle ratio for the two completely stirred tank step aeration system.

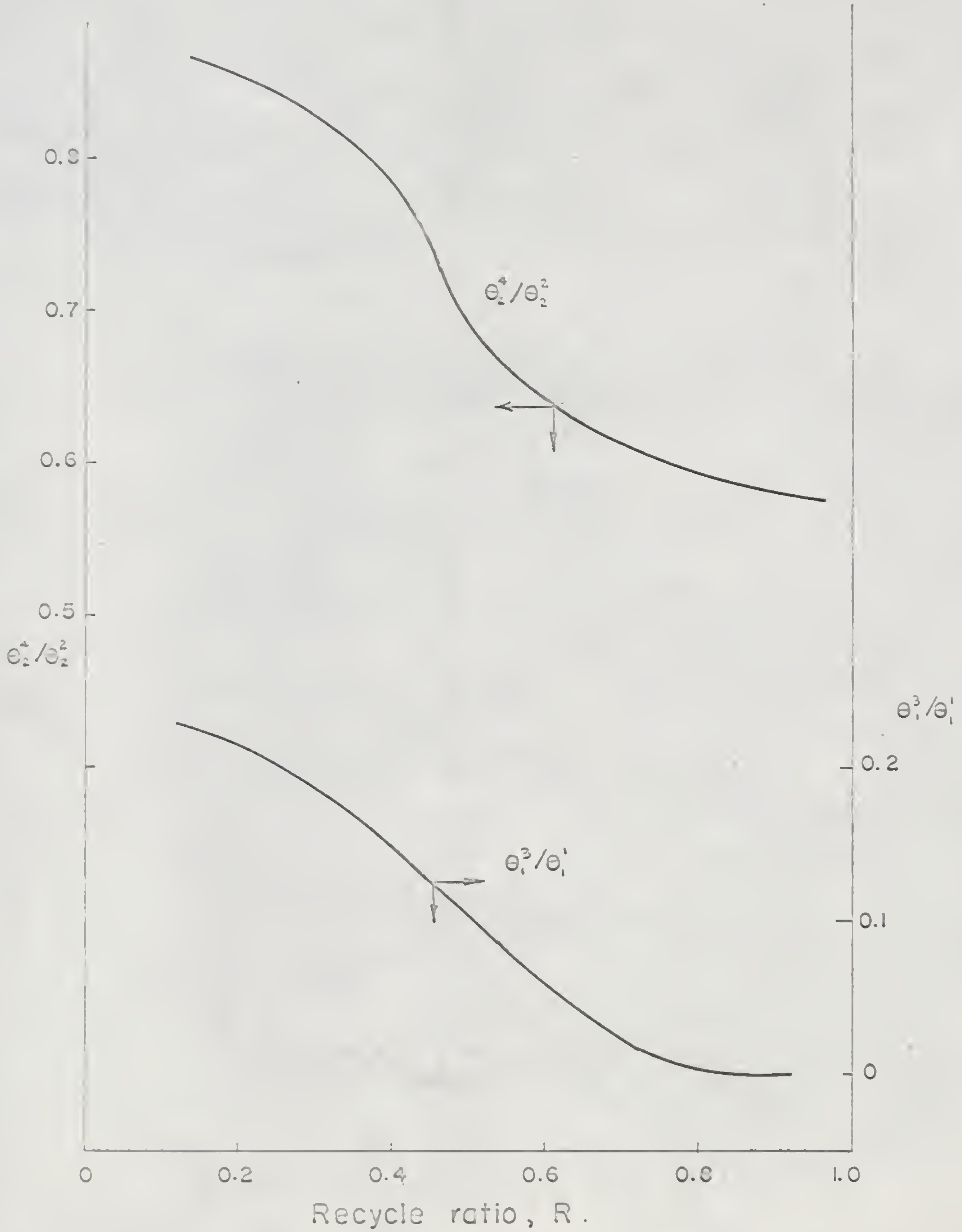


Fig. 18. Optimal feed distribution ratio and volume distribution ratio as function of recycle ratio for the two tank step aeration system.

3. OPTIMIZATION STUDIES OF STEP AERATION SYSTEMS CONSISTING OF SEVERAL PLUG FLOW REACTORS IN SERIES

As mentioned previously, the method of feeding the influent to the aeration system and the flow behavior are important variables in the step aeration process which affect the optimal design of the process. In this section an aeration system with no longitudinal mixing is considered and the optimal distribution of the organic load along the aeration system is examined with respect to its effect on the required aeration system volume. Since the undesirability of longitudinal mixing in the latter portion of the aeration system has already been pointed out, it is desirable to consider aeration systems with no longitudinal mixing.

As in the previous study, the system will be divided into mixing stages and reaction stages shown in Figures 6, 7 and 8 of Chapter 2; however, this time plug flow is assumed in the reaction stages. The material balance equations which describe the mixing and the growth process have been presented in Chapter 2.

(1) Formulation of the Problem

The problem is to find the optimal allocation of influent and the optimal distribution of volume between allocations for carrying out the waste treatment process in an aeration system represented by a sequence of plug flow reactors so that the total aeration system volume is minimized. The objective function of this problem can be represented as

$$S = x_3^{2N} \tag{35}$$

where x_3^{2N} represents the total aeration system volume.

The mathematical equations which describe this system are almost the same as those of the continuous stirred tank reactor in series system except for the reaction sections. The performance equations for the mixing stages are identical with those mentioned in the previous sections, that is, Equations (12), (13), and (14). The performance equations for the reaction stages are established as follows: From Equation (2.15), the overall material balance gives

$$x_1^{2n} = x_1^{2n-1} \ . \tag{36}$$

From Equation (2.30), the material balance of the oxidizable organics gives

$$\theta_2^{2n} = - \left[\frac{k}{ac} + \frac{1}{Yc} \right] \ell n \frac{(a - Yx_2^{2n-1})}{(a - Yx_2^{2n})} - \frac{K}{ac} \ \ell n \left(\frac{x_2^{2n}}{x_2^{2n-1}} \right) \tag{37}$$

Equation (37) can be functionally expressed as

$$x_2^{2n} = f\ (x_1^{2n-1},\ x_2^{2n-1},\ \theta_2^{2n})\ . \tag{38}$$

From Equation (18), the accumulated volume is

$$x_3^{2n} = x_3^{2n-1} + \theta_2^{2n}\ . \tag{39}$$

and thus, the objective function is

$$S = x_3^{2N}\ . \tag{40}$$

The optimization problem is thus one in which we wish to choose the allocation to each mixing stage and the volume of each reaction stage so that we minimize Equation (40) subject to the equality constraints given by Equations (12), (13), and (14) for the mixing stages and Equations (36), (37), and (39) for the reaction stages. It is assumed that the flow rates and concentrations of organics and organisms are known for the sludge recycle and influent streams, and that the outlet concentration of the organics is fixed.

The solution to this optimization problem can also be obtained by using the discrete maximum principle. As in the previous problem, we introduce adjoint variables and a Hamiltonian function for each stage. The Hamiltonian function and adjoint variables for mixing stages are given in Equations (19), (21), (23), (24), and (25). The Hamiltonian function for the reaction stages is

$$H^{2n} = z_1^{2n} x_1^{2n} + z_2^{2n} x_2^{2n} + z_3^{2n} x_3^{2n}$$

where x_1^{2n}, x_2^{2n}, and x_3^{2n} are given by Equations (36), (38), and (39) respectively. For the reaction stages, the adjoint variables can be obtained by diferentiating Equations (36), (37), and (39) with respect to x_j^{2n-1} for j = 1, 2, 3, and substituting the results into Equation (22). Thus the adjoint variables are given as

$$z_1^{2n-1} = z_1^{2n} + \frac{1}{B}\left[\frac{A_o(a + kY)(x_2^{2n-1} - x_2^{2n})}{ac(x_1^{2n-1})^2 (a - Yx_2^{2n})(a - Yx_2^{2n-1})}\right.$$

$$- \frac{KY\, x_1^{2n-1}(2A_o + Yx_2^f x_1^{2n-1})}{K_s^{max}(A_o + Yx_2^f x_1^{2n-1})^2} \ln \frac{x_2^{2n}(a - Yx_2^{2n-1})}{x_2^{2n-1}(a - Yx_2^{2n})}$$

$$\left. - \frac{1}{K_s^{max}} \ln \frac{a - Yx_2^{2n-1}}{a - Yx_2^{2n}}\right] , \tag{41}$$

where

$$B = \frac{K}{acx_2^{2n}} + \frac{a + KY}{ac(a - Yx_2^{2n})} \tag{42}$$

$$z_2^{2n-1} = z_2^{2n} \frac{1}{B}\left[\frac{a + KY}{ac(a - Yx_2^{2n})} + \frac{K}{acx_2^{2n-1}}\right] , \tag{43}$$

$$z_3^{2n-1} = z_3^{2n} \; . \tag{44}$$

Equations (25) and (44) reduce to $z_3^{2n-1} = z_3^{2n} = 1$, $n = 1, 2, \ldots, N$, since according to the maximum principle the boundary conditon for this adjoint variable is given as $z_3^{2N} = 1$.

The necessary conditions for a stationary point can be obtained by using the so-called weak form of the discrete maximum principle as given by Equation (6). For the mixing stages, this gives Equation (33) which has been obtained previously; however for the reaction stages, differentiating Equation (36), (37), and (39) with respect to θ_2^{2n} and substituting the results into Equation (32) gives

$$\frac{\partial H^{2n}}{\partial \theta_2^{2n}} = - \frac{z_2^{2n}}{B} + 1 = 0, \quad n = 1, 2, \ldots, N. \tag{45}$$

(2) Computational Scheme

The computational scheme for obtaining numerical solutions which was discussed previously can also be used to solve this set of nonlinear algebraic equations. However, the step in which we solve for x_2^{2n} is no longer straightforward and a numerical method such as the Regula Falsi method or Bolzano's method must be used. In this work, the Regula Falsi method was used. The computer program for the numerical solutions is given in Appendix 2.

(3) Results and Discussion

Numerical results which give the optimal influent distribution and the optimal volume distribution for a step aeration system consisting of several plug flow reactors connected in series are presented in this section. A simple approach to attain a best continuous influent distribution along a tublar reactor is qualitatively considered and discussed in the last portion of this section. In this numerical study, the kinetic constants are assigned the following values: $Y = 0.5$ mg/mg, $K = 100$ mg/l, $k^{s}_{max} = 0.1\ hr^{-1}$. The following additional conditions are also specified: $R = 0.4$, $x_2^0 = 150$ mg/l, $x_3^0 = 8000$ mg/l, $x_2^f = 800$ mg/l, $x_2^{2N} = 80$ mg/l, $\sum_{n=1}^{N} \theta_1^{2n-1} = 4500$ l/hr. Numerical solutions have been obtained using these data for step aeration systems consisting of one, two and three plug reactors connected in series. The results are listed in Table 6 and plotted in Figure 19. The lower curve which represents the results for the plug flow systems shows that the total required aeration system volume decreases exponentially as the number of feed locations in the system is increased. However, the reduction in volume obtained by adding other feed locations is small for cases with more than two feed locations. This shows that the effect of the influent distribution on the required reactor volume is

Table 6. Optimal Operating Policies for a System Composed of a Sequence of Plug Flow Reactors

System	Stage Number n	Optimal Policies: feed allocation, mg/ℓ. θ_1^{2n-1}	Optimal Policies: reactor volume, liters θ_2^{2n}	Optimal Total Volume, liters
single stage	1	4500	9440	9440
two stages	1	1910	2643	
	2	2590	5715	8358
three stages	1	1050	1234	
	2	2500	4200	
	3	950	2861	8295

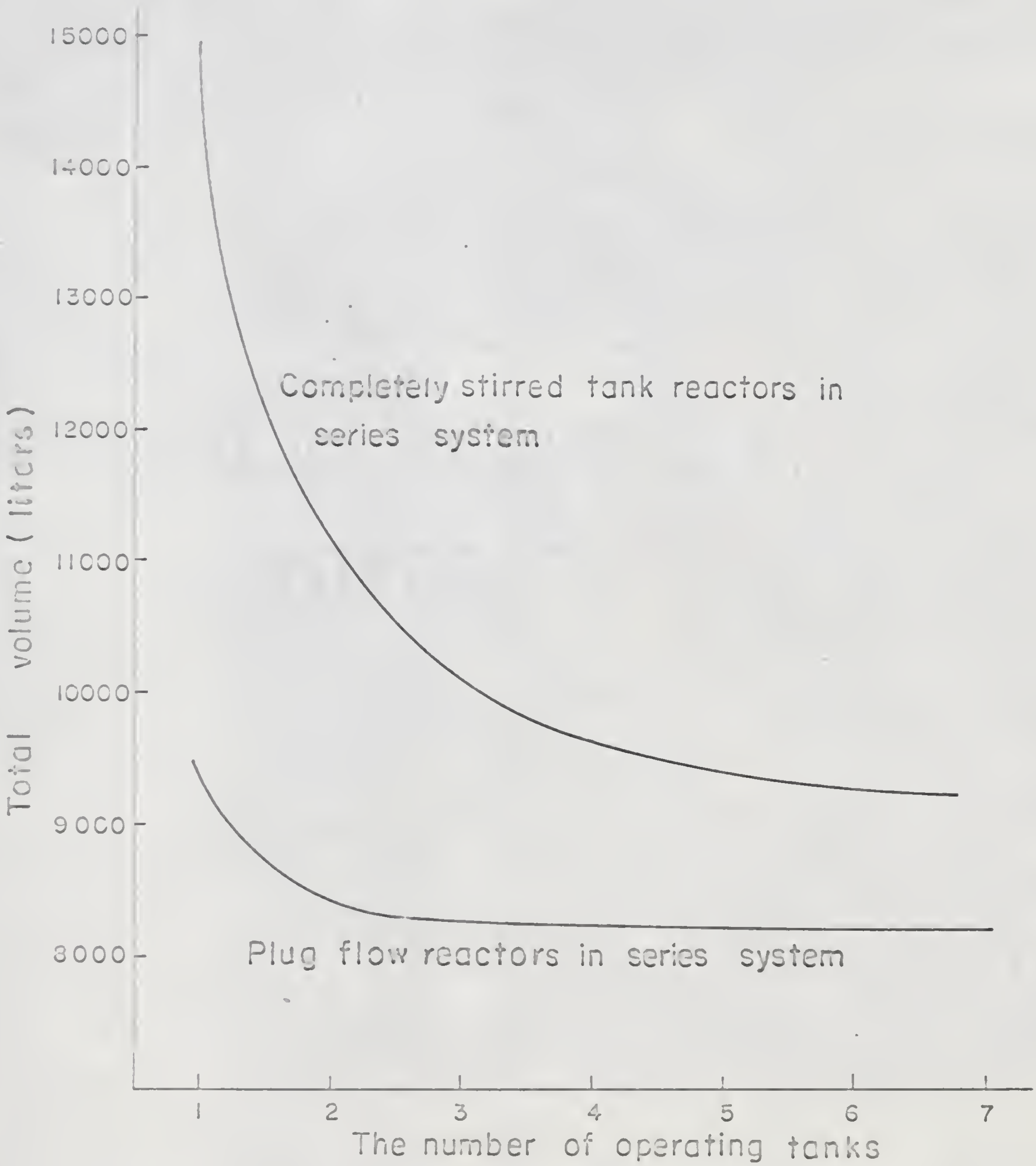


Fig. 19. Comparison of completely stirred tank reactor systems and plug flow reactor systems for step aeration process.

small for systems without longitudinal mixing. In Figure 19 the curve presented previously for the C.S.T.R. system is also plotted for comparison with the curve for the plug flow system. The two systems represent two extreme cases in that complete mixing is assumed in each tank of the C.S.T.R. in series system, while no longitudinal mixing is assumed for the plug flow reactor system. Other systems with incomplete mixing will lie between these two curves as shown in Figure 19.

In systems of plug flow reactors connected in series, the volume of each reactor and the quantity of influent added at the front of each reactor does not influence the longitudinal mixing in any way. On the other hand, in a system composed of a series of completely mixed tanks a change in the number of tanks or even the volume of one tank will change the mixing pattern of the system. In Figure 19 the decrease of required reactor volume with increasing stage number for the plug flow system is due only to the effect of changing the feeding pattern for the influent entering the system, while for the C.S.T.R in series system the decrease is due both to changes in the mixing pattern and to changes in the influent feeding pattern. Another graphical representation of these systems can also be made, and it is shown in Figure 20. The solid curves shown in Figure 20 are a plot of the reciprocal of the reaction rate versus the organic concentration with the

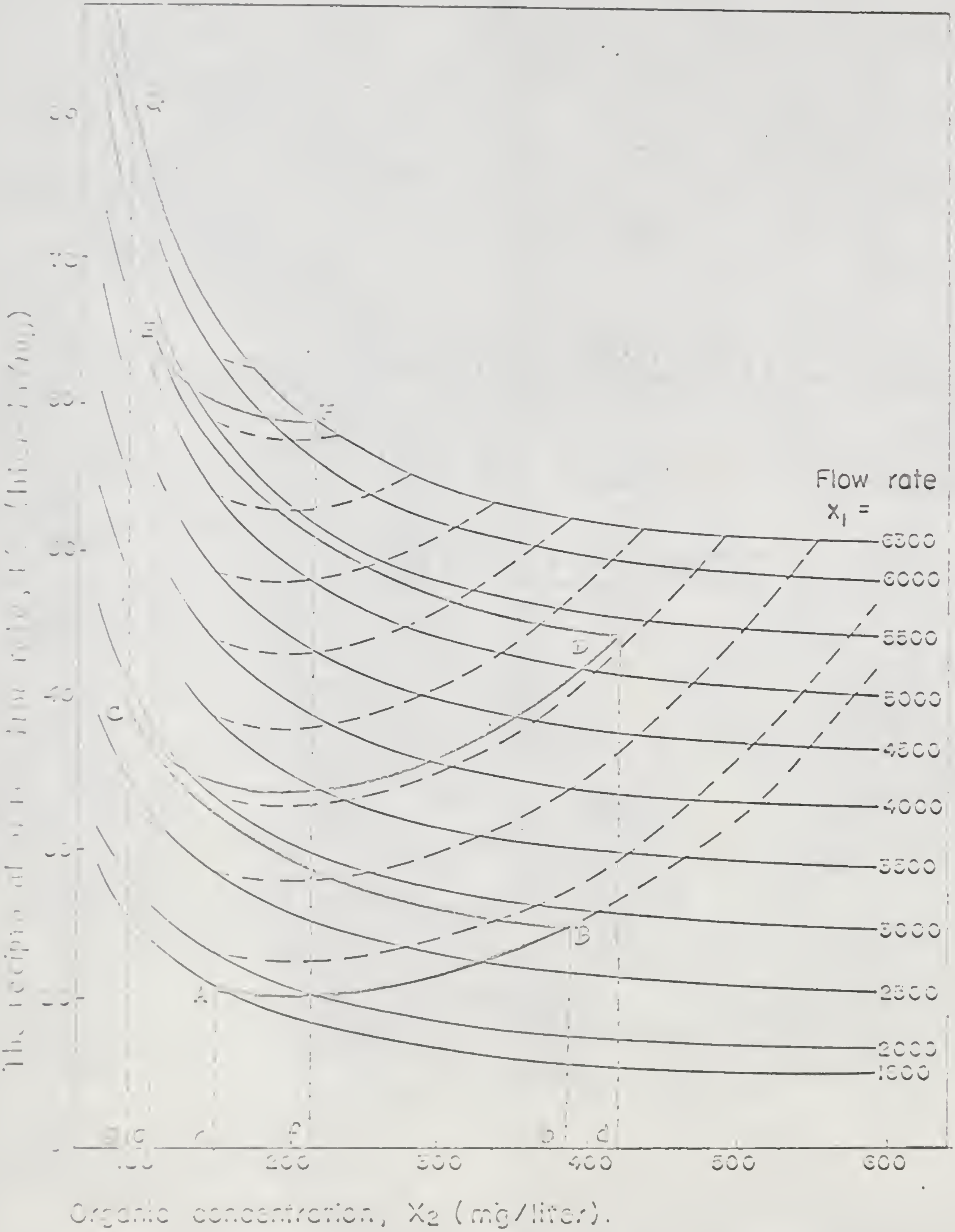


Fig. 20. Growth rate trajectory in an optimal three stage plug flow step aeration system.

flow rate as a parameter. The equation of the solid lines is obtained from equation (2.18), which is as follows

$$\frac{1}{r} \quad \frac{(K + x_2)}{k^s_{max}\, x_2 \quad (\frac{A_o}{x_1} + Yx_2^f - Yx_2)} \quad . \tag{46}$$

where

$$A_o = x_1^0\, x_4^0 + Y\, x_1^0\, x_2^0 - Y\, x_1^0\, x_2^f \; .$$

The dotted lines are determined from the mixing relation, equation (2.10), which can be written in the form

$$x_2^{2n-1} = x_2^f - \frac{x_1^{2n-2}\,(x_2^f - x_2^{2n-2})}{x_1^{2n-1}} \tag{47}$$

In Figure 20 the heavy solid line shows the path of the optimal locus of the three stage plug flow reactor in series system. The recycle stream is at point A, $x_1^0 = 1800$ and $x_2^0 = 150$. In the first stage where 1050 liters of influent are added to the recycle stream, curve AB up to point B is followed. As this material passes through the first reaction stage, the reaction curve BC is followed to point C. The area enclosed by bcCB represents the holding time required for the first reactor. In the same manner, the curve is followed up to D as 2500 liters of the second influent are added to the second mixing stage and then up to

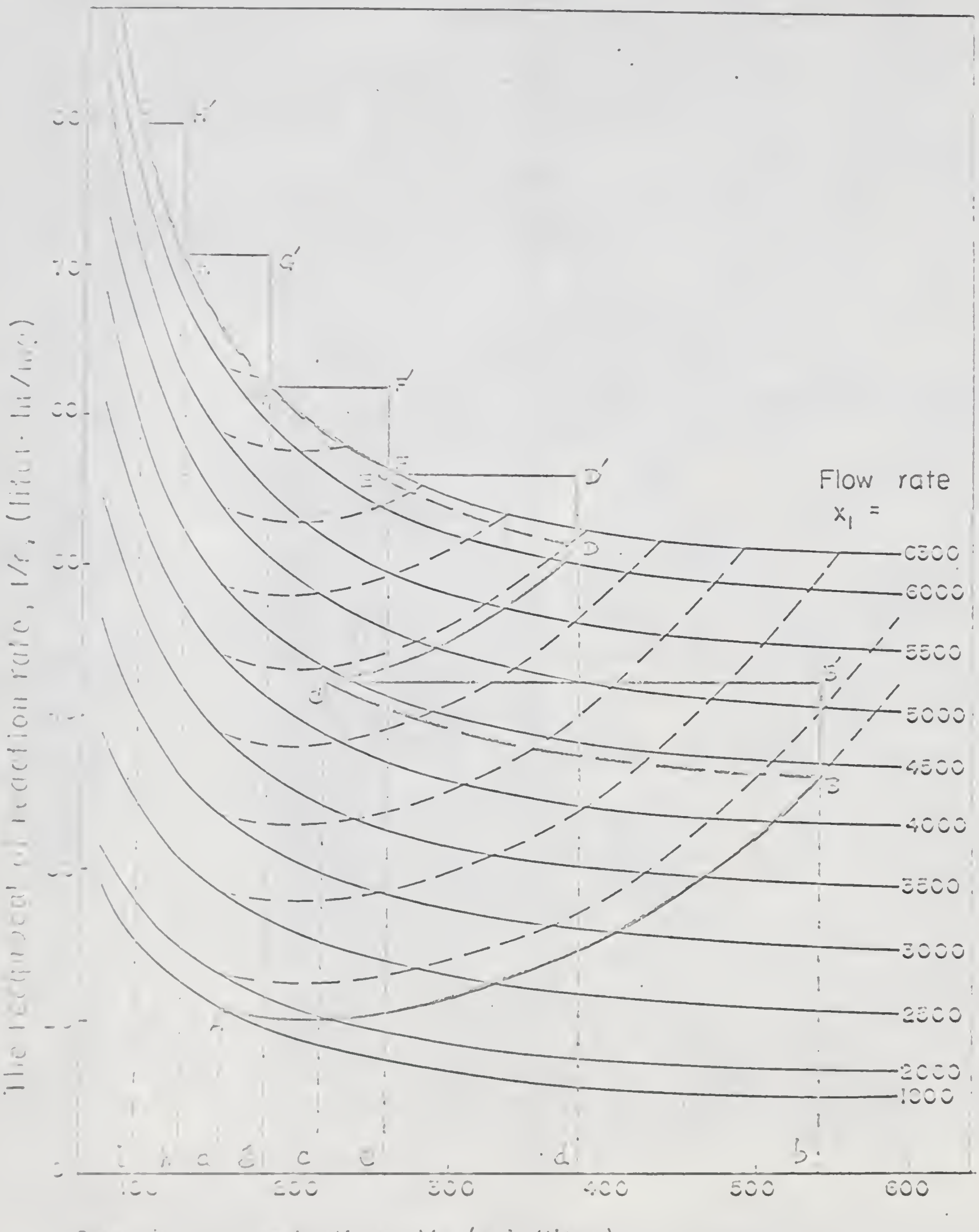


Fig. 21. Growth rate trajectory in an optimal five stage completely stirred tank step aeration system.

E as the material passes through the second reaction stage. Similarly for the last stage, the curve is followed up to F and then to G. Similarly, the areas enclosed by dDEe and fFGg represent the holding time required for the second and third reactor respectively. The total holding time is the sum of these three areas.

By using this graphical representation, the advantage of employing a plug flow reactor rather than a completely stirred tank flow reactor can be clearly illustrated. Based on the graph used in Figure 20, the optimal locus of the five completely stirred tanks in series system is plotted in Figure 21, i.e. the curve ABB'CDD'EFF'GG'HH'I. The total holding time will be the sum of the five rectangular areas; they are cbB'C edD'E, gfF'G, hgG'H and ihH'I. For the same influent flow situation and a plug flow reactor, the locus will be along ABCDFGHI. The areas, BCB', EDD', GFF', HGG', and IHH', represent the amount the holding time is reduced by using plug flow reactors instead of stirred tank reactors.

From a graphical analysis, we can see that a continuous feed allocation along a plug flow reactor which keeps the organic concentration at 200 mg/liter will yield the optimal policy for this system. In other words, the optimal locus will be the locus ABCD passing through the minimum points of the mixing lines as shown in Figure 22. A numerical result has been obtained by using a finite approximation of the continuous allocation system. In the

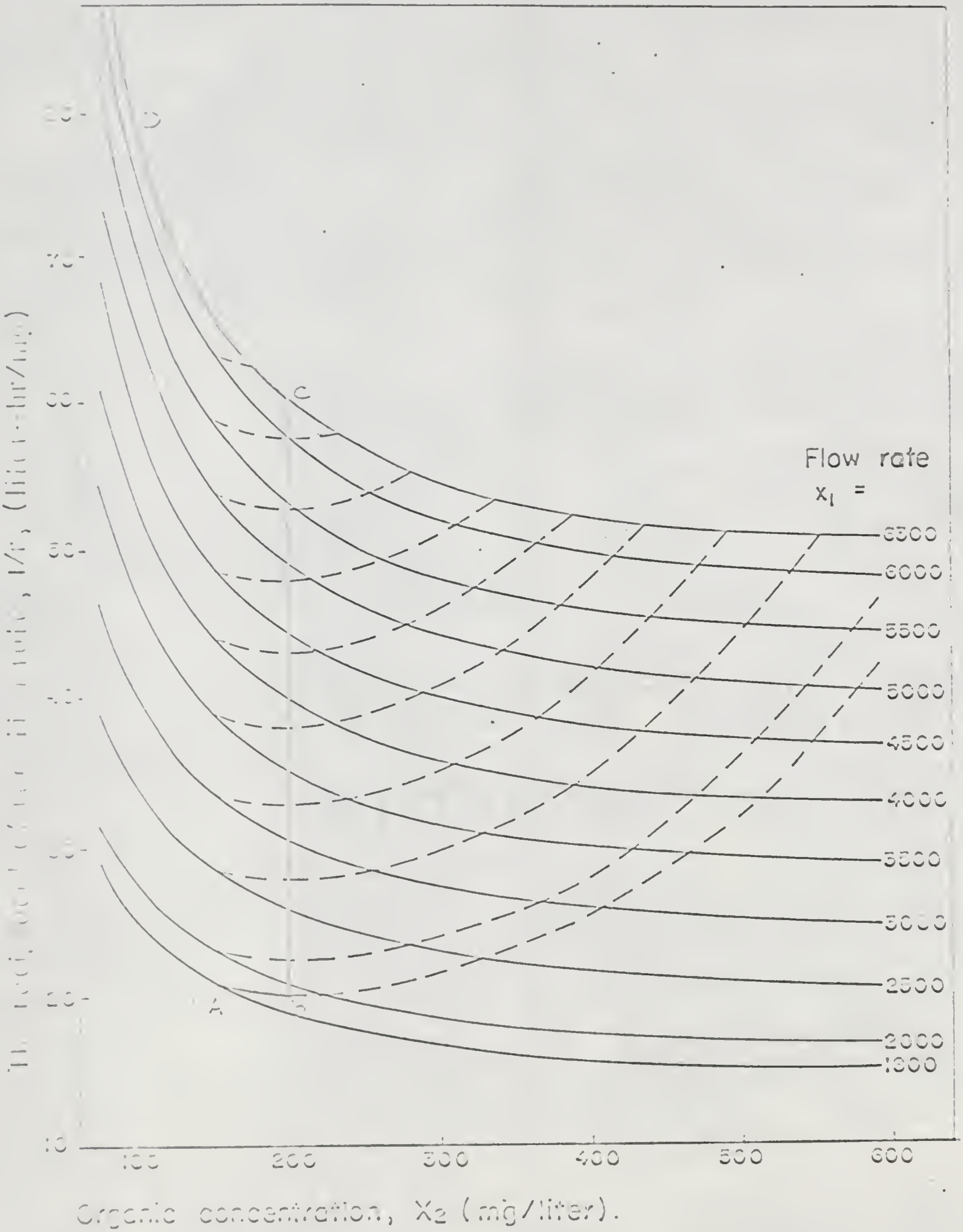


Fig. 22. Growth rate trajectory in a plug flow step aeration system with optimal allocation along the length of the system.

approximate system, influent is added at each mixing stage until an organic concentration of 200 mg/liter is reached. A 2% BOD reduction in each reaction stage is allowed; that is, the holding time is chosen so that the exit concentration from each plug flow reactor is 196 mg/liter. This pattern is followed until all of the influent has been added to the system. The total required volume by this approximate calculation is 8025.2 liters. This is an approximation to the limiting value of the two curves shown in Figure 18. When the number of tanks approaches infinity for either system, this limiting value is approached.

4. OPTIMIZATION STUDY OF COMPOSITE SYSTEM

From the standpoint of stability, use of a completely mixed tank reactor followed by a plug flow reactor may also be desirable. Because of this, we wish to investigate the behavior of a composite system under optimum conditions. The schematic diagram of the composite system is shown in Figure 23.

(1) Formulation of Problem

The problem is to find the optimal allocation of influent and the optimal distribution of volume for carrying out a waste treatment process in a composite step aeration system composed of a completely stirred tank reactor followed by a plug flow reactor. The allocation of influent and the

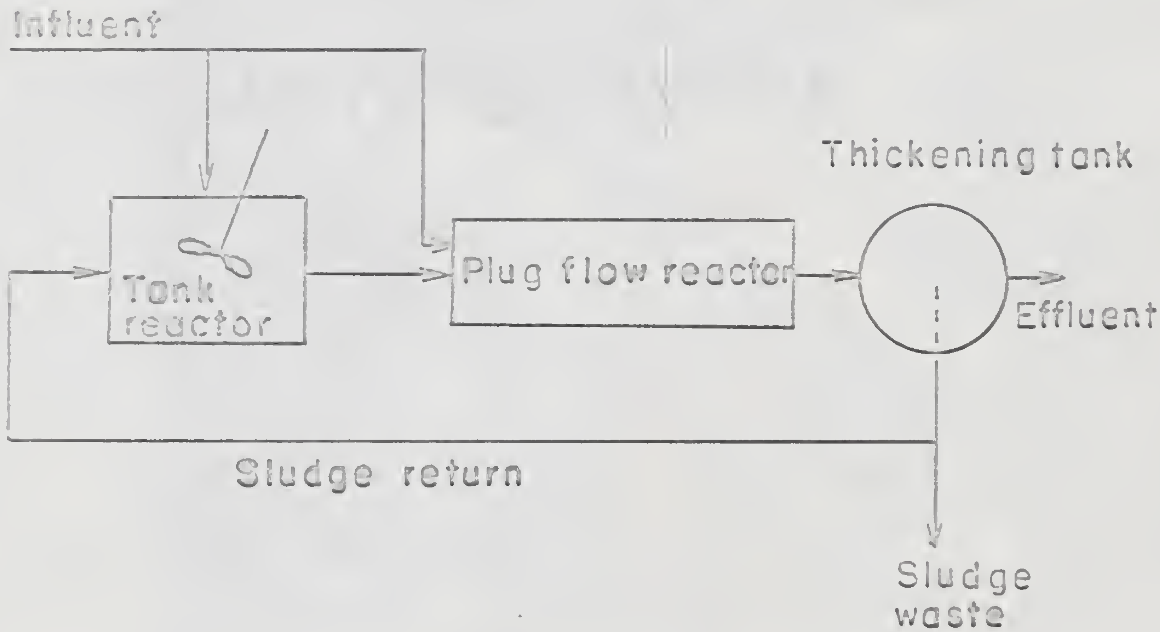


Fig. 23. Schematic diagram of composite system.

distribution of volume are to be chosen so that the total aeration system volume is minimized. The objective function of this problem is therefore the same as in previous systems and can be represented as

$$S = x_3^{2N} . \tag{48}$$

The mathematical equations which describe this system have been given previously as both systems have been discussed before. The performance equations for the mixing stages are Equations (12), (13), and (14). The performance equations for the reaction stages are Equations (15), (17), and (18) for the completely stirred tank reactor and Equations (36), (38), and (39) for the plug flow reactor.

This optimization problem can be solved by the discrete maximum principle. The adjoint equations and Hamiltonian function for n = 1 are the same as those for the completely stirred tank reactor system and are given by Equations (19) through (28). Those for the plug flow reactor system are given by Equations (41) through (44).

The computational scheme for obtaining numerical solutions which was discussed previously can also be used to solve this set of non-linear algebraic equations. The computer program which has been used to obtain the numerical solutions is given in Appendix 3.

(2) Results and Discussion

In this numerical study, the kinetic constants are assigned the following values: $Y = 0.5$ mg/mg, $K = 100$ mg/l, $k^s_{max} = 0.1\ hr^{-1}$. The following additional conditions are also specified: $R = 0.4$, $x^0_2 = 150$ mg/l, $x^0_3 = 8000$ mg/l, $x^f_2 = 800$ mg/l, $x^{2N}_2 = 80$ mg/l, $\sum_{n=1}^{N} \theta_1^{2n-1} = 4500$ l/hr.

The numerical result which gives the optimal influent distribution and the optimal value distribution for this system is given as follows:

$$\theta_1^1 = 1810\ \text{l/hr},$$
$$\theta_2^2 = 1790\ \text{liters},$$
$$\theta_1^3 = 2690\ \text{l/hr},$$
$$\theta_2^4 = 6956.5\ \text{liters},$$
$$V = \theta_2^2 + \theta_2^4 = 8746.5\ \text{liters}.$$

This result may be compared with the optimal result fo V = 8358.1 for two plug flow reactors connected in series. The reason that the result obtained using the composite system is not as good as that obtained using the two plug flow reactor system can be interpreted in Figure 24. In Figure 24 the optimal locus of the compostie system is represented by the curve ABCDEF. If for the same operating conditions the first completely stirred tank is replaced by a plug flow reactor, the optimal locus will be the curve ABDEF as shown in Figure 23; however, this is not the optimal

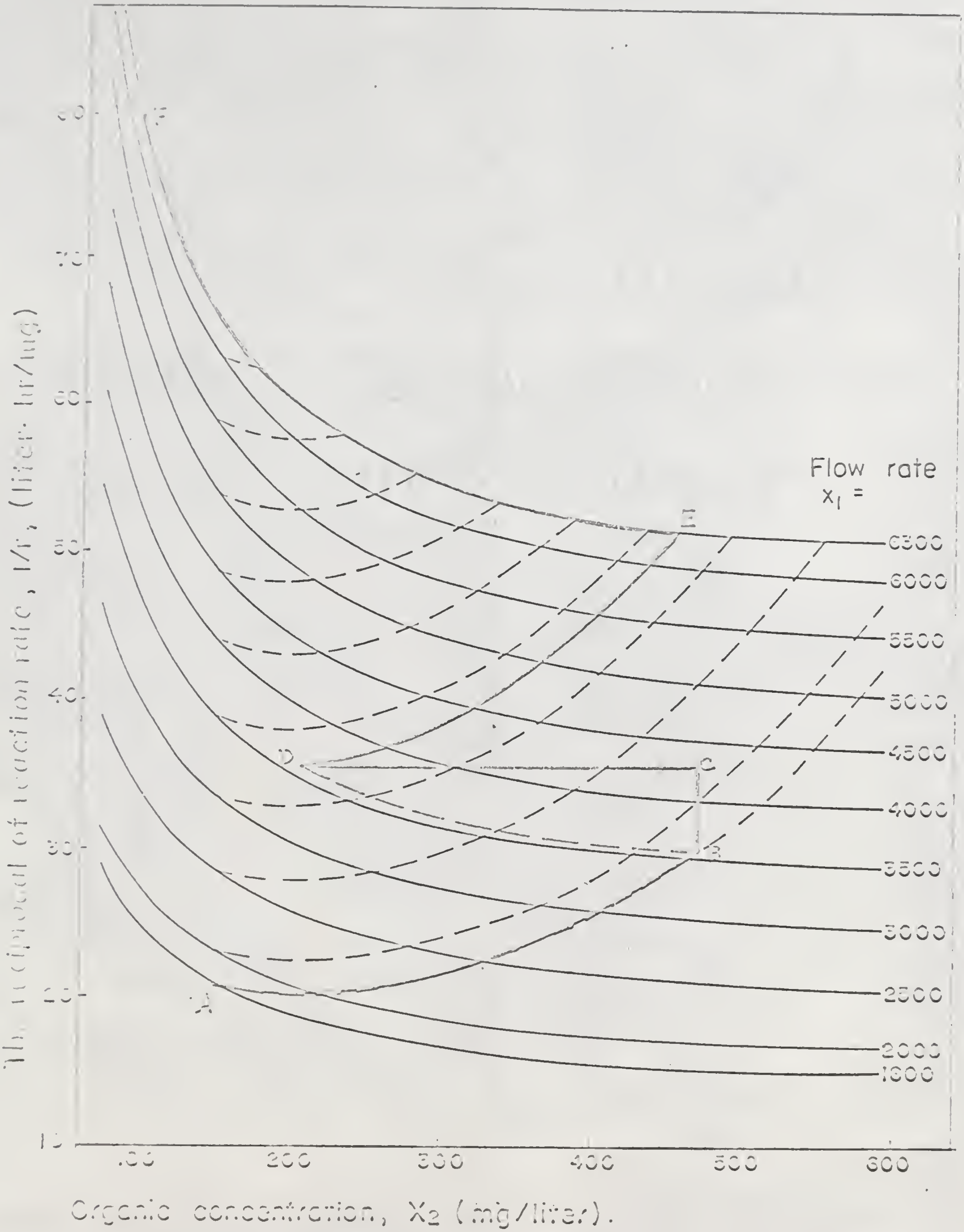


Fig. 24. Growth rate trajectory in an optimal composite step aeration system.

operating condition for two plug flow reactors connected in series. As described previously the area BCD will be the holding time saved by using two plug flow reactors rather than using the composite system.

The reason for often employing a tank reactor as the first reactor for an autocatalytic reaction has been discussed by Bischoff (11). It is used in an effort to increase the concentration of organisms and thus to attain the maximum reaction rate in the front part of the system. In our study a sufficient amount of organisms are contained in the recycle stream and thus it is not necessary to use a tank reactor.

CHAPTER V

CONCLUSION

In this study we have proposed several flow systems for use with the step aeration process. These systems include several completely stirred tank reactors in series, several plug flow reactors in series, and a composite system composed of a stirred tank reactor and a plug flow reactor. Under simplifying assumptions, the optimum operating conditions have been determined by using the maximum principle and a search technique.

In general, from the optimization studies the allocation of feed along the system is found to be desirable under the conditions that are considered in this study. In other words, the step aeration system is theoretically desirable in some types of operating situations.

From all the systems we have considered, we have found that a continuous feed allocation along a plug flow system is the optimal policy for the step aeration system. Under the situations and assumptions of this study, the plug flow system is far better than the completely mixed flow system. We have also found from the study of the composite system that plug flow is most necessary at the back end and that complete mixing does not increase the volume requirements very much at the front end of the step aeration system.

The numerical data and the kinetic constants employed in this study may not be of practical significance. However, better experimental data and more refined kinetic models can be easily incorporated into the scheme developed in this study to obtain more realistic results. A more realistic flow model can also be used instead of the idealized reactors we have considered.

NOMENCLATURE

Symbol

A	Cross-section area, cm^2 .
H^n	Hamiltonian function at the nth stage.
k^s_{max}	Maximum growth rate when the organics is unlimited, hr^{-1} .
K	Growth rate constant, mg/liter.
L	Total length of a plug flow reactor, cm .
ℓ	Length of the reactor, cm .
r	Growth rate, mg/l-hr .
R	Recycle ratio
S	Objective function
s	concentration of organics, mg/liter .
x	Concentration of organisms, mg/liter .
x^n_1	Volumetric flow rate of the flow discharged from the nth stage, l/hr .
x^n_2	Concentration of organics in the inlet stream of the nth stage, mg/liter .
x^n_3	Accumulated volume up to the nth stage, liter .
x^n_4	Concentration of organisms in the inlet stream of the nth stage, mg/liter .
x^f_2	Concentration of organics in the feed, mg/liter .
x^f_4	Concentration of organisms in the feed, mg/liter .
Y	Yield factor
z^n_i	The ith adjoint variable at the nth stage.
α	Correction factor
θ^n_1	Volumetric flow rate of sewage introduced at the nth stage, l/hr .
θ^n_2	Reactor volume of the nth stage, liter .

PART TWO

AN OPTIMIZATION STUDY OF THE REVERSE OSMOSIS DESALINATION PROCESS

CHAPTER I

INTRODUCTION

Because of its simplicity and the potential low energy requirement, reverse osmosis has been drawing widespread attention. Current research activities have been directed to (A) development of membranes which combine good salt rejection, high water transmission at reasonable pressure, and long membrane life, (B) improvement of membrane fabrication techniques, (C) improvement of cell design and construction, and (D) mathematical and experimental studies of salt build-up on the membrane surface. However, only a rather limited attention has been directed to the system analysis of the entire system (12).

Recently, because of the thermodynamic undesirability of mixing a recycle stream of high salt concentration with another stream of much lower salt concentration, a multistage sequential system with brine recycle at each stage has been proposed (13). In order to increase the efficiency of energy recovery of this system, use of a flow work exchanger has been proposed by Cheng et al. (14).

The present study is directed to the mathematical modeling and optimization of the entire reverse osmosis system incorporating the improvements mentioned above. A combination of the discrete version of the maximum principle and the steepest descent search technique is used to carry out the optimization. This study illustrates how optimization can be used in a process design study which has an objective function based on the economics of the process.

CHAPTER II

DESCRIPTION OF PROCESS

1. REVERSE OSMOTIC PROCESS (15)

Much interest has been shown recently in reverse osmosis as a promising method for the economic recovery of water from saline sources. In reverse osmosis, desalination is achieved by forcing salt solution under pressure through a membrane which generally passes water much more readily than salts. The simplicity of the reverse-osmosis process is apparent upon inspection of a flow sheet of the Aerojet pilot plant (16). Basically the process consists of a pumping system to raise the pressure of the brine solution and of an array of selective membranes. The only energy consumption required by the process is that for driving the pumps. A reduction in energy consumption will reduce the cost of the fresh water produced.

Water passing through the membrane is supplied to the membrane boundary by bulk flow of solution normal to the membrane. Salt is carried along with the water. If a steady state is to be maintained without an accumulation of salt on the membrane, this salt must diffuse back into the main bulk solution. A salt concentration gradient is established near the membrane boundary such that the net salt flux normal to the membrane is zero. This means that the salt concentration and osmotic pressure are greater at the membrane than in the bulk solution. If we use a circulation pump to obtain fully developed turbulent flow inside the tubes, the bulk of the brine flowing parallel to the osmotic membrane surface will be well mixed, and the existence of concentration and velocity gradients will be restricted to the laminar boundary layer as shown in Figure 1.

Based upon this boundary layer model, the desired performance equation which relates the applied pressure, circulation rate, and the flux of the fresh water produced has been developed (13, 15) in detail.

2. DESCRIPTION OF MULTISTAGE PROCESS (13)

As mentioned in the introduction, because of the thermodynamic undesirability of mixing a recycle stream of high salt concentration with a main stream of lower salt concentration, a multistage process has been proposed (13). In order to increase the efficiency of the purification caused by the stagewise increase in salt concentration, the use of a pressure pump between successive stages has also been suggested. Figure 2 illustrates the proposed sequential purification process.

The process is a form of a simple sequential multistage model as shown in Figure I-13. Each stage, except the last one, consists of a membrane separator unit, a

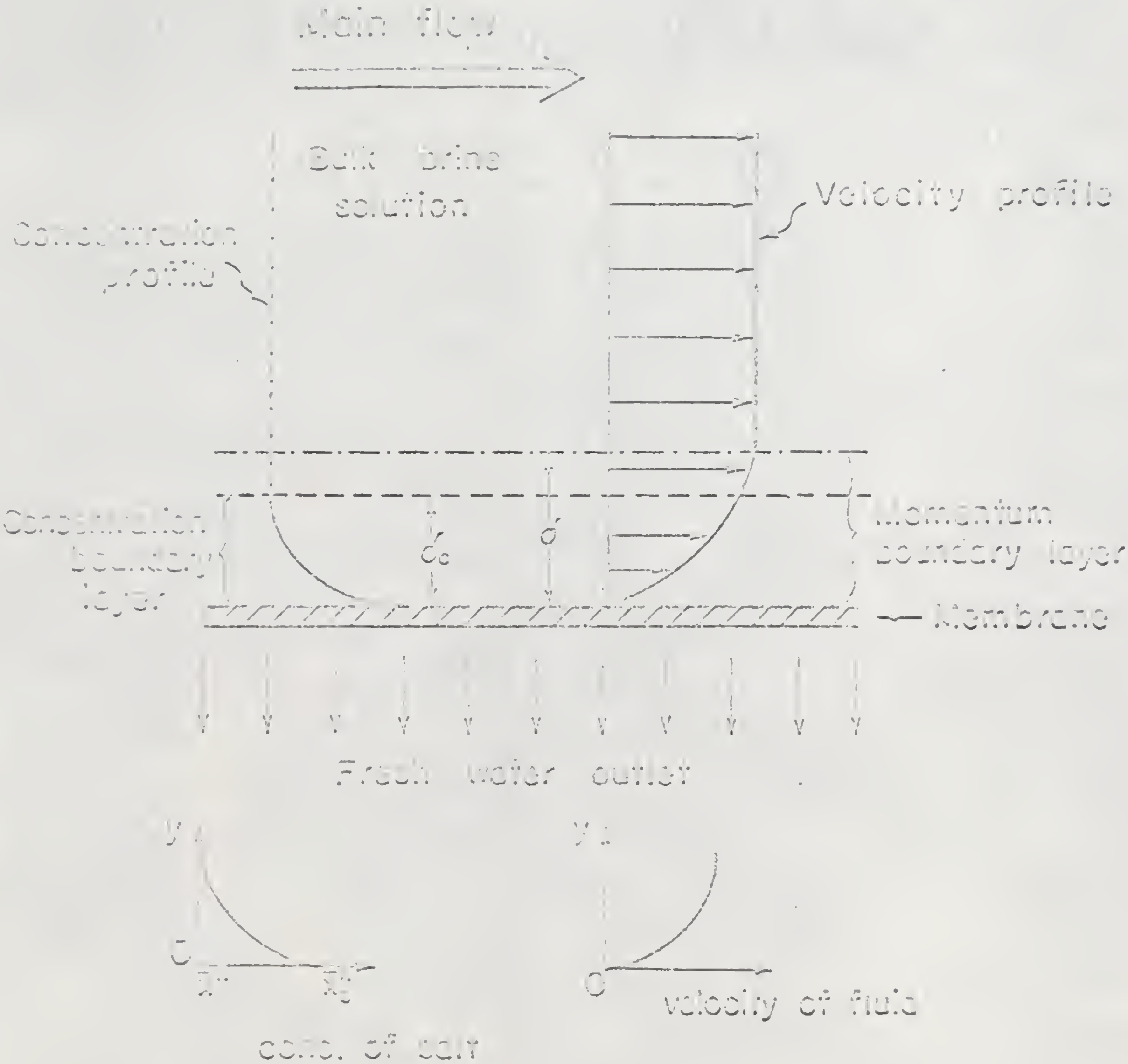


Fig. 1. Velocity and salt concentration gradients in boundary layer adjacent to a membrane.

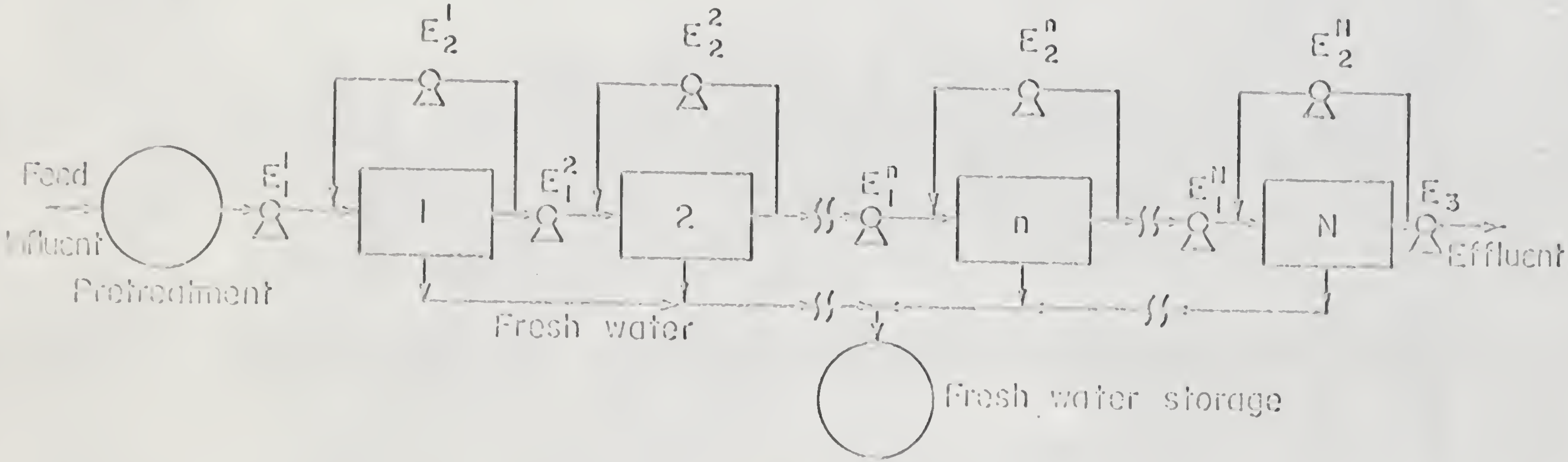


Fig. 2. Schematic diagram of a sequential conventional reverse osmosis water purification process.

Where: E_1^n: the high pressure pump at n^{th} stage.

E_2^n: the circulation pump at n^{th} stage.

E_3: the [illegible] at [illegible] of the process.

recycle unit and a high pressure pump unit. The last stage is similar to the others but adds one turbine unit in its outlet for energy recovery. When a flow work exchanger is incorporated into the proposed sequential process; it is connected between the first and the last stage as shown in Figure 3.

In setting up these models, the following assumptions have been made.

(a) The flow model is fixed, but the geometric parameters of the membrane separator unit itself, i.e., the pipe diameter d, length-to-diameter ratio L/D, and the total number of tubes used, m, are chosen arbitrarily.

(b) The salt concentration in the fresh water produced is assumed to be zero, i.e., the salt cannot pass through the membrane.

(c) The saline water feed solution contains 3.5 weight per cent salt.

(d) There is no precipitation of salt on the membrane surface.

(e) The costs of the pump, turbine, and motor are assumed to be directly proportional to horsepower rating in the horsepower range of interest.

(f) The cost of the membrane separator unit is proportional to the weight of the material used.

(g) D_a, μ, and ρ are assumed to be constant in the concentration range of interest.

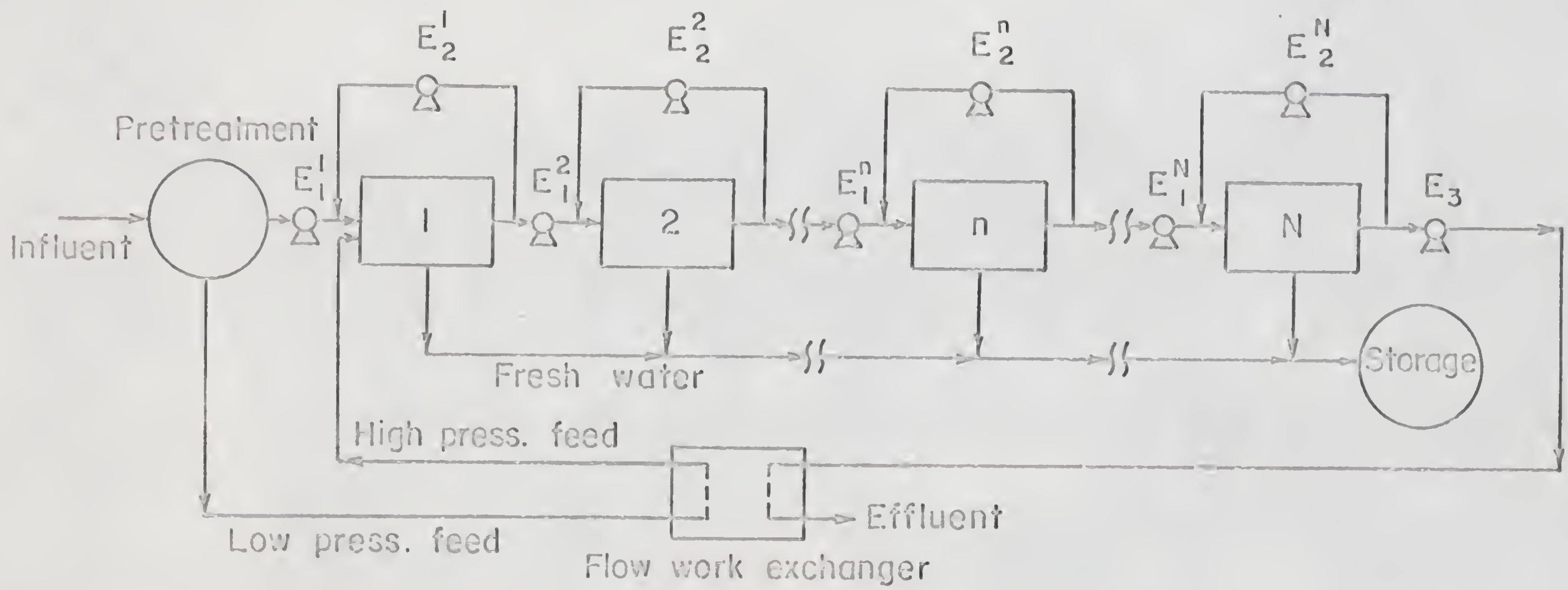


Fig. 3. Schematic diagram of a sequential reverse osmosis water purification process using flow work exchanger.

Where E_1^n : the high pressure pump at n stage.

E_2^n : the circulation pump at n stage.

E_3 : the flowdown turbine at the end of the process.

(h) Membrane constant K is assumed to be independent of pressure.

Process and cost analyses for the multistage reverse osmosis process have been developed previously (13). We now simply summarize these relations as follows:

(I) Process Analysis

The equation for the fresh water flux at the nth stage is

$$F^n = \frac{K(\Delta p^n - 12100\ \bar{x}^n)}{1 + c\ \dfrac{\bar{x}^n}{(Re^n)^{7/8}}}$$

where

$$c = 3.05 \times 10^5\ \frac{Kd}{(Sc)^{1/3} D_a} \quad ,$$

K = the membrane constant $\dfrac{ft^3}{ft^2\text{-}hr\text{-}psi}$

Δp^n = the pressure difference across the membrane of the nth stage, psi.

Re^n = the average Reynolds number at the nth stage,

Sc = Schmidt number,

d = the diameter of the tubes in the membrane separator unit, ft,

D_a = molecular diffusion coefficient of salt, $\dfrac{\text{Sq cm}}{\text{Sec}}$,

$\bar{x}^n$ = the average mass fraction of salt at the nth stage.

The overall material balance and the salt balance around the nth stage give

$$q^n = q^{n-1} - W^n = q^{n-1} - F^n \rho S^n \ , \qquad (2)$$

and

$$q^o x^o = q^n \bar{x}^n \ , \qquad (3)$$

where

q^n, q^{n-1} = the mass flow rate of the brine solution discharged from the nth, (n-1) stage, $\frac{lb_m}{hr}$.

q^o = the mass flow rate of the inlet brine solution, $\frac{lb_m}{hr}$.

W^n = the mass flow rate of fresh water product from the nth stage, $\frac{lb_m}{hr}$.

ρ = the density of the fresh water, $\frac{lb_m}{ft^3}$.

S^n = the membrane area of the nth stage, ft^2.

x^o = the inlet mass fraction of sea water.

Combining Equations (8) and (9) and using a salt balance to eliminate q^{n-1} gives

$$x^n = \frac{c^o x^o}{q^n} = \frac{x^o \ x^{n-1}}{x^o - x^{n-1} \ F^n \ \rho(\frac{S^n}{q^o})} \ . \qquad (4)$$

(II) Cost Analysis

The total cost required for the system mainly consists of the operating and capital costs. These costs are separately summarized in Section A and B below.

A. Operating cost:

The energy requirement for the high pressure pump at the nth stage per pound of total fresh water produced is

$$\frac{E_1^n}{W_f} = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{\Delta p^n - \Delta p^{n-1}}{\rho} \cdot \frac{x^o}{x^{n-1} \left(1 - \frac{x^o}{x^N}\right)} \tag{5}$$

where

η_m, η_p, η_r = the mechanical, pump, and turbine efficiencies,

η_f = the loss factor,

W_f = Total mass flow rate of fresh water produced from the system, lb_m/hr .

The energy requirement for the recycle pump at the nth stage per pound of total fresh water produced is

$$\frac{E_2^n}{W_f} = 0.023 \, (Re^n)^{2.8} \left(\frac{\mu}{d\rho}\right)^3 \frac{S\rho}{q^o \left(1 - \frac{x^o}{x^N}\right)} \frac{1 + \eta_f}{g_c \eta_m \eta_p} \tag{6}$$

The energy recovery at the reject-brine turbine per pound of total fresh water produced is

$$\frac{E_3}{W_f} = \eta_p \eta_m (1 - \eta_f) \frac{\Delta p^N}{\rho} \frac{x^o}{x^N - x^o} . \tag{7}$$

If a flow-work exchanger is used, the turbine is only used to recover energy as the pressure is reduced from Δp^N to Δp^1. The flow work exchanger is in turn used to transfer energy to the feed. An amount q^N of sea water is pressurized in the first stage with this energy. Therefore, the energy recovery per pound of total fresh water produced becomes

$$\frac{E_3}{W_f} = \eta_p \eta_m (1 - \eta_f) \frac{\Delta p^N - \Delta p^1}{\rho} \frac{x^o}{x^N - x^o} . \tag{8}$$

Because of the flow work exchanger, the energy requirement for the high pressure pump at the first stage is simply to pump the amount of $q^o - q^N$ rather than q^o. Therefore,

$$\frac{E_1^1}{W_f} = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{\Delta p^1}{\rho} \frac{q^o - q^N}{W_f} , \tag{9}$$

Since

$$W_f = q^o - q^N ,$$

$$\Delta p^o = 0,$$

Equation (9) becomes

$$\frac{E_1^1}{W_f} = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{\Delta p^1}{\rho} . \tag{10}$$

Here all the energy required is assumed to be supplied from electricity and the electrical power cose, C_e, is assumed to be \$0.007 per Kw-hr for all cases.

B. Capital cost:

For simplicity the cost of pump, turbine, and motor are assumed to be directly proportional to horsepower rating in the horsepower range of interest.

The membrane separator cost is assumed to be proportional to the weight of the material used. The weight of the material used per pound of the fresh water produced for this unit has been suggested to be

$$\frac{W_s^n}{W_f} = \frac{\rho_m d}{\sigma_m} \frac{S \Delta p^n}{q^o \left(1 - \frac{x^o}{x^N}\right)} \left(1.62 + \frac{0.54}{L/D} + \frac{0.189}{L/D} \sqrt{\frac{\sigma_m}{\Delta p^n}}\right) \qquad (11)$$

where

ρ_m = the density of the material of construction, $\frac{lb_m}{ft^3}$,

W_s^n = the mass of the shell-and-tube membrane separator unit of the nth stage, lb_m,

σ_m = the allowable stress of the material of construction, psi,

L/D = the overall length-to-diameter ratio of the membrane separator unit.

In the final cost estimation by Lonsdale et al. (15), f.o.b. costs of \$50/Kw were assumed for the circulation pump with motor, and the blowdown turbine, an f.o.b. cost of \$100/Kw was assumed for the high-pressure pump, and an f.o.b. cost of \$4.40/lb for the separator unit. As recommended in the Office of Saline Water Procedures (17), f.o.b. costs should be multiplied by 1.3 to obtain installed costs. It also recommended that interest on the depreciated plant investment be at 4%, and depreciation be over 20 years. This gives a total charge of 7.4% for amortization on the initial investment. In addition to the above items, two per cent is added for taxes and insurance. This gives an annual capitalization charge for these equipment items of 9.4% of the initial cost. Then an assumption of a load factor of 330-on-stream days per year gives a capitalization charge of 11.94×10^{-6} of initial cost per hour on stream, ψ.

C. Total cost:

Combining both the operating and capital costs, the total cost contribution of the system is obtained in the form

$$C_T = (\psi C_{pH} + C_e) \sum_{n=1}^{N} \frac{E_1^n}{W_f} + (\psi C_{pR} + C_e) \sum_{n=1}^{N} \frac{E_2^n}{W_f}$$

$$+ (\psi C_{pT} - C_e) \frac{E_3}{W_f} + \psi C_s \sum_{n=1}^{N} \frac{W_s^n}{W_f} \qquad (12)$$

where C_{pH}, C_{pR}, C_{pT}, and C_s are respectively the capital costs of the high-pressure pump, circulation pump, turbine, and separator unit.

Substituting Equations (5), (6), (7), and (11) into Equation (12) and combining all constants, we obtain

$$C_T = B_1 \frac{x^o}{1 - \frac{x^o}{x^N}} \sum_{n=1}^{N} \frac{\Delta p^n - \Delta p^{n-1}}{x^{n-1}} + \left(\frac{x^N}{x^N - x^o}\right)$$

$$\cdot \left[B_2 \sum_{n=1}^{N} (Re^n)^{2.8} \left(\frac{s^n}{q^o}\right) + B_3 \sum_{n=1}^{N} \Delta p^n \left(\frac{s^n}{q^o}\right) + B_4 \sum_{n=1}^{N} (\Delta p^n)^{\frac{1}{2}} \left(\frac{s^n}{q^o}\right)\right]$$

$$+ B_5 \frac{x^o}{x^N - x^o} \Delta p^N \qquad (13)$$

where

$$B_1 = (\psi C_{pH} + C_e) \frac{1 + \eta_f}{\eta_m \eta_p} ,$$

$$B_2 = 0.023 \; (\psi C_{pR} + C_e) \frac{1 + \eta_f}{g_c \eta_m \eta_p} \left(\frac{\mu}{d \rho}\right)^3$$

$$B_3 = \frac{C_s \rho_m d}{\sigma_m} \left(1.62 + \frac{0.54}{L/D}\right) ,$$

$$B_4 = \frac{0.189 \; C_s \rho_m d}{\sigma_m \; L/D} ,$$

$$B_5 = (\psi C_{pT} - C_e) \, \eta_p \, \eta_m \, (1 - \eta_f)/\rho .$$

When a flow work exchanger is employed, we can combine Equations (6), (8), (10), (11), and (12) to obtain

$$C_T = B_1 \Delta p^1 + B_1 \frac{x^o}{1 - \frac{x^o}{x^N}} \sum_{n=2}^{N} \frac{\Delta p^n - \Delta p^{n-1}}{x^{n-1}}$$

$$+ \left(\frac{x^N}{x^N - x^o}\right) \left[B_2 \sum_{n=1}^{N} (Re^n)^{2.8} \left(\frac{s^n}{q^o}\right) + B_3 \sum_{n=1}^{N} \Delta p^n \left(\frac{s^n}{q^o}\right) \right.$$

$$\left. + B_4 \sum_{n=1}^{N} (\Delta p^n)^{\frac{1}{2}} \left(\frac{s^n}{q^o}\right) \right] + B_5 \frac{x^o}{x^N - x^o} (\Delta p^N - \Delta p^1)$$

$$+ B_6 \frac{x^o}{x^N - x^o} \; p^N \quad . \tag{14}$$

where

$$B_6 = \frac{1}{\rho} (\psi C_{pF} + \xi C_e) \; .$$

Here we assume that the capital cost of the flow work exchanger, C_{pF}, is the same as that of turbine and use to denote the inefficiency of the device.

CHAPTER III

OPTIMIZATION STUDY OF THE PROCESS

In Chapter II the equations which describe the performance of the reverse osmosis process are given. Cost equations which relate these performance equations to the unit cost of product water are also given.

In this chapter these performance equations and cost equations are used together with optimization techniques to determine the values of the design variables that minimize the cost of producing a given quantity of fresh water.

In the present study we classify the optimization studies of the reverse osmosis system into the following two classes of problems:

(1) Multistage operation without the use of a flow work exchanger,

(2) Multistage operation with the use of a flow work exchanger.

As in Part I, the discrete maximum principle is also employed here. The discrete maximum principle has been briefly described in Part I.

1. MULTISTAGE OPERATION WITHOUT FLOW WORK EXCHANGER

(1) Formulation of the Problem

The optimization problem will be formulated so that it conforms to the "standard" notation and structure of a discrete maximum principle optimization problem. Figure 4

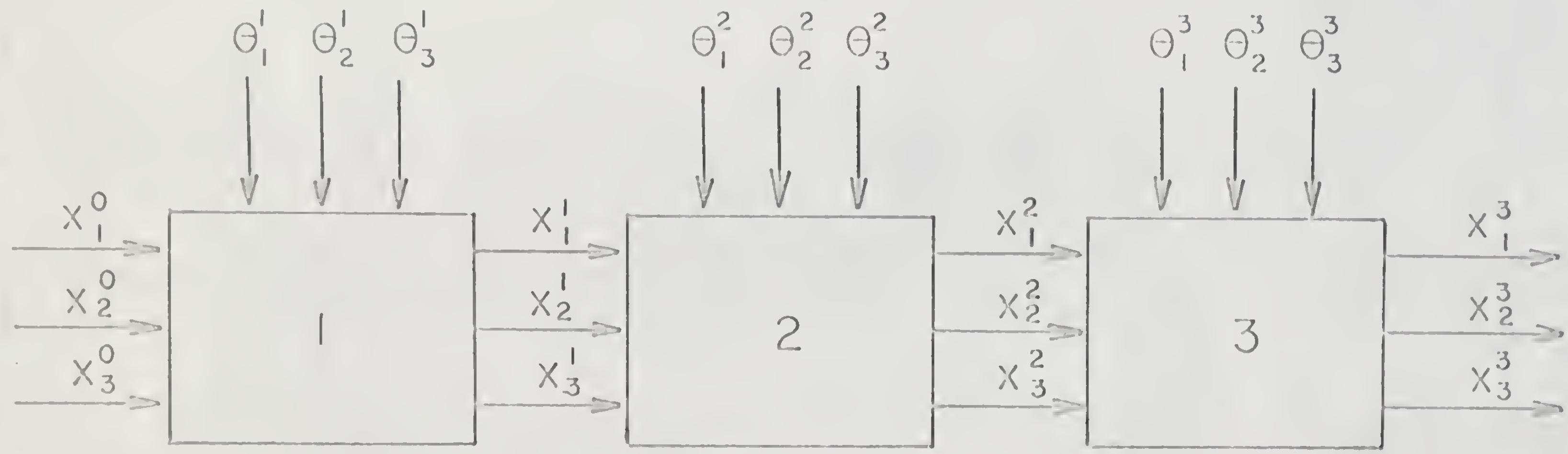


Fig. 4 Discrete Maximum Principle Model of the Reverse Osmosic System

illustrates the structure of the sequential three stage discrete maximum principle model of the reverse osmosis system without the flow work exchange that is shown in Figure 2. In Figure 4 two types of variables are indicated. Those represented by are decision variables which are treated as independent variables, while those represented by x are state variables which are dependent variables. Superscripts are used to denote the stage with which each variable is associated. The state and decision variables are defined as follows:

(a) State variables

x_1^n = salt concentration at the nth stage,

x_2^n = total cost required up to and including the nth stage.

(b) Decision variables

$\theta_1^n = \Delta p^n$, the pressure difference across the membrane of the nth stage,

$\theta_2^n = Re^n$, the average Reynolds number at the nth stage,

$\theta_3^n = \frac{s^n}{q^o}$, the ratio of membrane area and inlet mass flow rate at the nth stage.

From Equation (2.4) we can see that the performance equation for the first state variable, x_1^n, can be expressed as

$$y^n = y^{n-1} - \frac{K\rho}{x_1^0}\left[\frac{\theta_1^n\, y^n - 12100}{y^n + \dfrac{c}{(\theta_2^n)^{7/8}}}\right]\theta_3^n\,, \quad n = 1, 2, \ldots, N. \tag{1}$$

where

$$y^n = \frac{1}{x_1^n} \tag{2}$$

The performance equation for the second state variable x_2^n, can be obtained from Equation (2.13) as

$$x_2^n = x_2^{n-1} + A_1 y^{n-1}\,(\theta_1^n - \theta_1^{n-1}) + A_2\theta_3^n\left[B_2(\theta_2^n)^{2.8} + B_3(\theta_1^n) + B_4(\theta_1^n)^{\frac{1}{2}}\right], \quad n = 1, 2, \ldots, N-1, \tag{3}$$

$$x_2^N = x_2^{N-1} + A_1 y^{N-1}\,(\theta_1^N - \theta_1^{N-1}) + A_2\theta_3^N\left[B_2(\theta_2^N)^{2.8} + B_3(\theta_1^N) + B_4(\theta_1^N)^{\frac{1}{2}}\right] + A_3\theta_1^N\,, \tag{4}$$

Since Equations (3) and (4) have memory in decision θ_n^{n-1}, for simplification, we can introduce the new state variable, x_3^n such that

$$x_3^n = \theta_1^n\,, \quad n = 1, 2, \ldots, N. \tag{5}$$

Equations (3) and (4) then become

$$x_2^n = x_2^{n-1} + A_1 y^{n-1} (\theta_1^n - x_3^{n-1}) + A_2 \theta_3^n \; B_2(\theta_2^n)^{2.8} + B_3 \theta_1^n$$

$$+ B_4(\theta_1^n)^{\frac{1}{2}} \quad , \qquad n = 1,\ 2,\ \ldots,\ N\text{-}1, \tag{6}$$

$$x_2^N = x_2^{N-1} + A_1 y^{N-1} (\theta_1^N - x_3^{N-1}) + A_2 \theta_3^N \; B_2(\theta_2^N)^{2.8} + B_3 \theta_1^N$$

$$+ B_4(\theta_1^N)^{\frac{1}{2}} + A_3 \theta_1^N, \tag{7}$$

where

$$A_1 = B_1 \frac{x_1^0}{1 - \dfrac{x_1^0}{x_1^N}} \tag{8}$$

$$A_2 = \frac{x_1^N}{x_1^N - x_1^0} \tag{9}$$

$$A_3 = B_3 \frac{x_1^0}{x_1^N - x_1^0} \quad . \tag{10}$$

We are to find the optimal design variables that minimize the total required cost of producing a given quantity of fresh water. The objective function of this problem is therefore simply represented as

$$S = x_2^N \ . \tag{11}$$

In applying a discrete from of the maximum principle to determine the optimal policy for the system as described above, the following Hamiltonian functions and adjoint are introduced

$$H^n = z_1^n y^n + z_2^n x_2^n + z_3^n x_3^n , \tag{12}$$

$$z_1^{n-1} = \frac{\partial H^n}{\partial y^{n-1}} = z_1^n \frac{\partial y^n}{\partial y^{n-1}} + z_2^n \frac{\partial x_2^n}{\partial y^{n-1}} + z_3^n \frac{\partial x_3^n}{\partial y^{n-1}} , \tag{13}$$

$$z_2^{n-1} = \frac{\partial H^n}{x_2^{n-1}} = z_1^n \frac{\partial y^n}{\partial x_2^{n-1}} + z_2^n \frac{\partial x_2^n}{\partial x_2^{n-1}} + z_3^n \frac{\partial x_3^n}{\partial x_2^{n-1}} , \tag{14}$$

$$z_3^{n-1} = \frac{\partial H^n}{\partial x_3^{n-1}} = z_1^n \frac{\partial y^n}{\partial x_3^{n-1}} + z_2^n \frac{\partial x_2^n}{\partial x_3^{n-1}} + z_3^n \frac{\partial x_3^n}{\partial x_3^{n-1}} . \tag{15}$$

Differentiating Equations (1), (6), (7), and (5) with respect to y^{n-1}, x_2^{n-1}, and x_3^{n-1}, and substituting the results into Equations (13), (14) and (15) respectively, we obtain

$$z_1^{n-1} = z_1^n \frac{(G)^2}{(G)^2 + k_1 \theta_3^n \left[\frac{c_1^n}{(\theta_2^n)^{7/8}} + 12,100 \right]} + z_2^n A_1 (\theta_1^n - x_3^{n-1}) \tag{16}$$

where

$$G = y^n + \frac{c}{(\theta_2^n)^{7/8}} , \quad n = 1, 2, \ldots, N, \tag{17}$$

$$z_2^{n-1} + z_2^n \,, \quad n = 1, 2, \ldots, N, \tag{18}$$

$$z_3^{n-1} = z_2^n A_1 y^{n-1} \,, \quad n = 1, 2, \ldots, N. \tag{19}$$

Since x_1^N is specified, the boundary conditions for the adjoint variables in this system are

$$z_2^N = 1, \tag{20}$$

$$z_3^N = 0. \tag{21}$$

According to the so-called weak form of the discrete maximum principle, the optimal decision variables at each stage must satisfy the equations

$$\frac{\partial H^n}{\partial \theta_i^n} = z_1^n \frac{\partial v^n}{\partial \theta_i^n} + z_2^n \frac{\partial x_2^n}{\partial \theta_i^n} + z_3^n \frac{\partial x_3^n}{\partial \theta_i^n} = 0, \quad \begin{array}{l} i = 1, 2, 3. \\ n = 1, 2, \ldots, N. \end{array} \tag{22}$$

where

$$\frac{\partial v^n}{\partial \theta_1^n} = \frac{-K_1 y^n \left[y_1^n + \frac{c}{(\theta_2^n)^{7/8}} \right] \theta_3^n}{\left[y_1^n + \frac{c}{(\theta_2^n)^{7/8}} \right]^2 + K_1 \theta_3^n \left[\frac{c\theta_1^n}{(\theta_2^n)^{7/8}} + 12100 \right]} \,, \tag{23}$$

$n = 1, 2, \ldots, N.$

$$\frac{\partial v^n}{\partial \theta_2^n} = \frac{-7\, cK_1 \theta_3^n (y_1^n \theta_1^n - 12100)}{8(\theta_2^n)^{15/8}\left[\left(y_1^n + \frac{c}{(\theta_2^n)^{7/8}}\right)^2 + K_1\theta_3^n\theta_1^n \left(y_1^n + \frac{c}{(\theta_2^n)^{7/8}}\right) - K_1\theta_3^n(y_1^n\theta_1^n - 12100)\right]}, \qquad n = 1, 2, \ldots, N, \tag{24}$$

$$\frac{\partial v^n}{\partial \theta_3^n} = \frac{K_1\ (\theta_1^n\ y^n - 12100)}{\left[y^n + \frac{c}{(\theta_2^n)^{7/8}}\right] + K_1\theta_3^n \left[\frac{\frac{c_1^n}{(\theta_2^n)^{7/8}} + 12100}{y^n + \frac{c}{(\theta_2^n)^{7/8}}}\right]} \tag{25}$$

$n = 1, 2, \ldots, N.$

$$\frac{\partial x_2^n}{\partial \theta_1^n} = A_1 y^{n-1} + A_2 B_3\, \theta_3^n + \tfrac{1}{2}\, A_2 B_4\, \theta_3^n (\theta_1^n)^{-\frac{1}{2}}, \qquad n = 1, 2, \ldots, N - 1. \tag{26}$$

$$\frac{\partial x_2^N}{\partial \theta_1^N} = A_1 y^{N-1} + A_2 B_3\, \theta_3^N + \tfrac{1}{2}\, A_2 B_4 \theta_3^N (\theta_1^N)^{-\frac{1}{2}} + A_3, \tag{27}$$

$$\frac{\partial x_2^n}{\partial \theta_2^n} = 2.8\ A_2 B_2\ (\theta_3^n)\ (\theta_2^n)^{1.8}, \qquad n = 1, 2, \ldots, N. \tag{28}$$

$$\frac{\partial x_2^n}{\partial \theta_3^n} = A_2 \left[B_2(\theta_2^n)^{2.8} + B_3\,\theta_1^n + B_4(\theta_1^n)^{\frac{1}{2}} \right], \quad n = 1, 2, \ldots, N. \tag{29}$$

$$\frac{\partial x_3^n}{\partial \theta_1^n} = 1, \qquad n = 1, 2, \ldots, N. \tag{30}$$

$$\frac{\partial x_3^n}{\partial \theta_2^n} = 0, \qquad n = 1, 2, \ldots, N. \tag{31}$$

$$\frac{\partial x_3^n}{\partial \theta_3^n} = 0, \qquad n = 1, 2, \ldots, N. \tag{32}$$

(2) Results and Discussion

The computational scheme for carrying out the optimization of the sequential multistage problem with some end points fixed as described in Part I can be applied to this problem.

Numerical computation has been performed with an IBM 1620 computer. A computer diagram to carry out a three stage problem is shown in Figure 5. A computer program is given in Appendix 4.

The following data are chosen for this study:

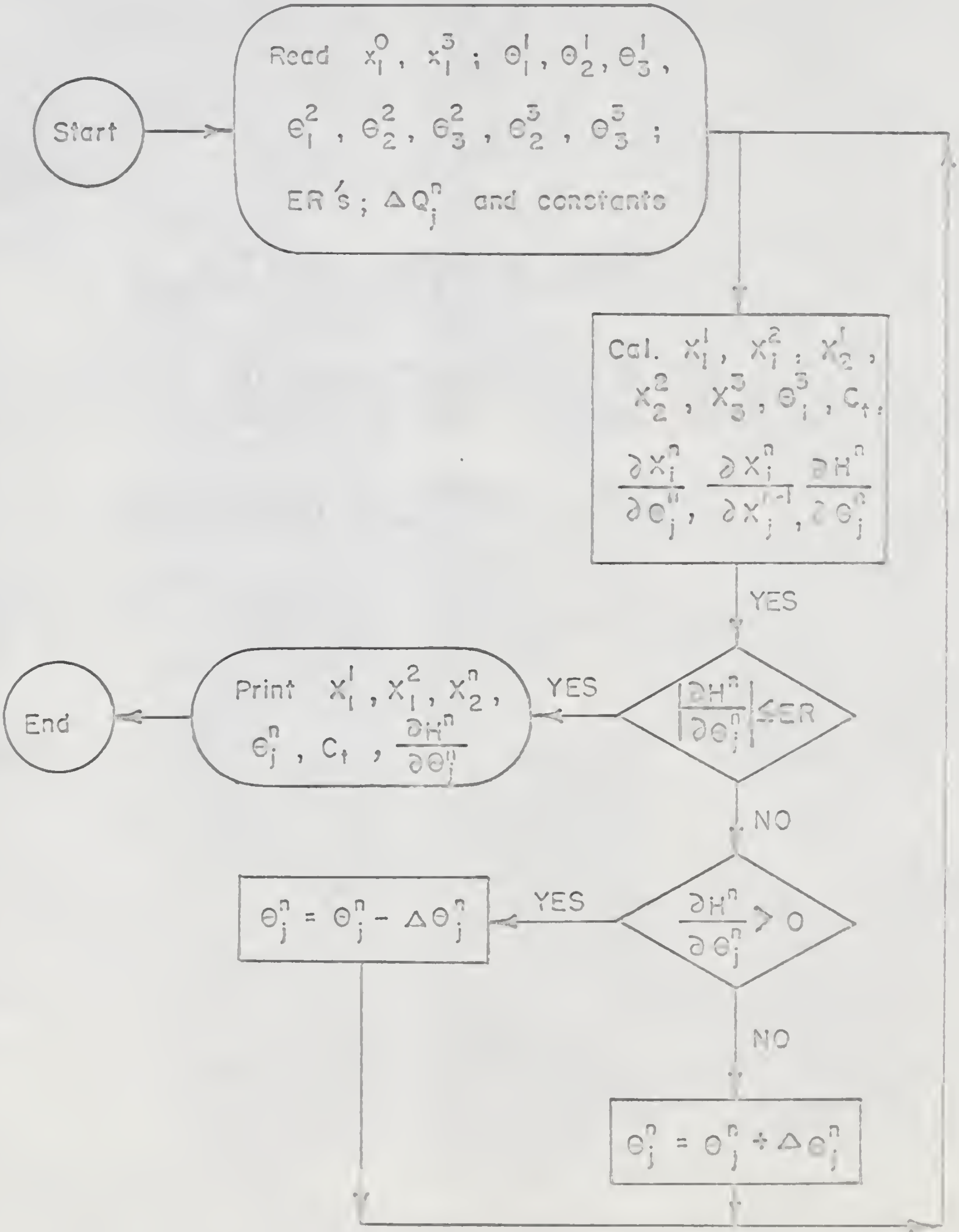


Fig.5. Computer flow diagram

D_a $= 1.5 \times 10^{-5} \frac{cm^2}{sec}$, the diffusion constant for sodium chloride in water at room temperature,

K $= 0.86 \times 10^{-4} \frac{ft^3}{ft^2\text{-hr-psi}}$,

ν $= 8 \times 10^{-3} \frac{cm^2}{sec}$ for the brines at 30°C,

ρ $= 62.4 \frac{lb_m}{ft^3}$,

d $= \frac{1}{24}$ ft.,

$\frac{L}{D}$ $= 8$,

ρ_m $= 2.7 \times 62.4 \frac{lb_m}{ft^3}$, density of aluminum,

σ_m = 15000 psi, allowable stress of aluminum,

ψ $= 11.94 \times 10^{-6}\ hr^{-1}$,

C_{pH} $= 100 \frac{\$}{KW}$ f.o.b.,

C_{pT} $= 50 \frac{\$}{KW}$ f.o.b.,

C_{pR} $= 50 \frac{\$}{KW}$ f.o.b.,

C_S $= 4.4 \frac{\$}{lb_m}$ of aluminum f.o.b.,

C_e $= 0.007 \frac{\$}{Kw\text{-hr}}$,

η_m $= 0.9$,

η_r $= \eta_p = 0.8$,

η_f $= 0.1.$

ξ $= 0.1.$

The related constants are, therefore,

$$Sc^{\frac{1}{3}} = \left(\frac{\nu}{D_a}\right)^{\frac{1}{3}} = 8.1,$$

$$c = \frac{3.05 \times 10^5 \, Kd}{Sc^{1/3} D_a} = 2320,$$

$$B_1 = 0.1136 \times 10^{-7} \frac{\$}{psi\text{-}lb_m},$$

$$B_2 = 0.6330 \times 10^{-17} \frac{\$}{ft^2\text{-}hr},$$

$$B_3 = 0.52 \times 10^{-7} \frac{\$}{ft^2\text{-}hr},$$

$$B_4 = 0.1773 \times 10^{-6} \frac{\$}{psi\text{-}ft^2\text{-}hr},$$

$$B_5 = -0.3494 \times 10^{-8} \frac{\$}{lb_m\text{-}psi},$$

$$B_6 = 0.11238 \times 10^{-8} \frac{\$}{lb_m\text{-}psi}.$$

The numerical results are listed in Table 1. The optimal cost, optimal Reynolds number, optimal pressure drop, and optimal membrane area to feed rate ratio are plotted against the parameter, x_1^N, in Figures 6, 7, 8, and 9. From these figures we can find the overall optimal cost and the corresponding design variables. They are

$$\Delta P^1 = 1401.4, \quad \Delta P^2 = 1686.9, \quad \Delta P^3 = 1704.3,$$

$$Re^1 = 8802.0, \quad Re^2 = 9088.0, \quad Re^3 = 10030.0,$$

Table 1. Optimal Conditions for a Three Stage Reverse Osmosis Process without the Use of Flow Work Exchanger for Various Outlet Salt Concentrations

Outlet salt concentration x_1^N, mg/ℓ.	Pressure drop, Δp^n, psia			Reynolds number, Re^n			Membrane area to feed ratio, $S^n/q^o \times 10^{-2}$, ft^2-hr/lb_m			Total Cost, Ct, \$/1000 gal.
	1^{st}	2^{nd}	3^{rd}	1^{st}	2^{nd}	3^{rd}	1^{st}	2^{nd}	3^{rd}	
0.05	911.8	983.1	987.1	760.8	7902.2	8101.2	4.489	4.620	4.632	0.5221
0.06	1145.7	1201.6	1212.2	8081.2	8635.3	9082.9	4.742	4.693	4.620	0.4635
0.07	1236.3	1411.3	1411.5	8286.5	9064.8	9704.3	4.887	4.798	4.683	0.4457
0.08	1211.4	1556.8	1559.2	8121.8	9069.6	9748.2	5.253	5.211	5.060	0.4409
0.09	1401.4	1686.9	1704.3	8802.0	9088.0	10030.0	5.530	5.240	4.380	0.4397
0.10	1375.0	1812.0	1870.8	8900.0	10180.0	11320.0	7.100	5.000	3.840	0.4411
0.15	1530.0	2170.0	2763.6	10200.0	12800.0	15500.0	8.450	4.600	3.100	0.4625
0.18	1590.0	2355.0	3283.2	10525.0	13375.0	16875.0	8.950	4.550	2.650	0.4767

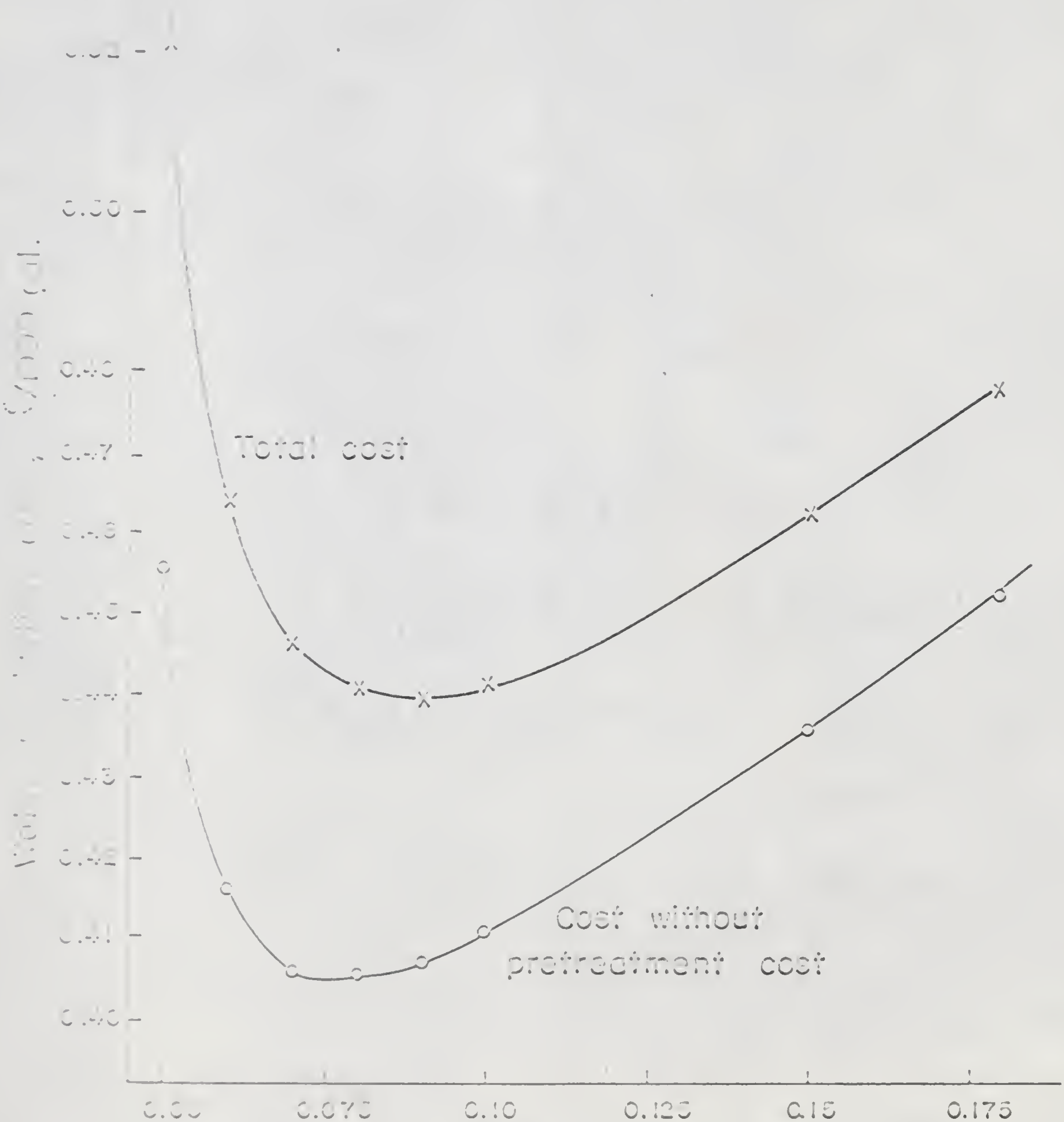


Fig. 5. Optimal water production cost vs. exit salt concentration for a conventional three stage system.

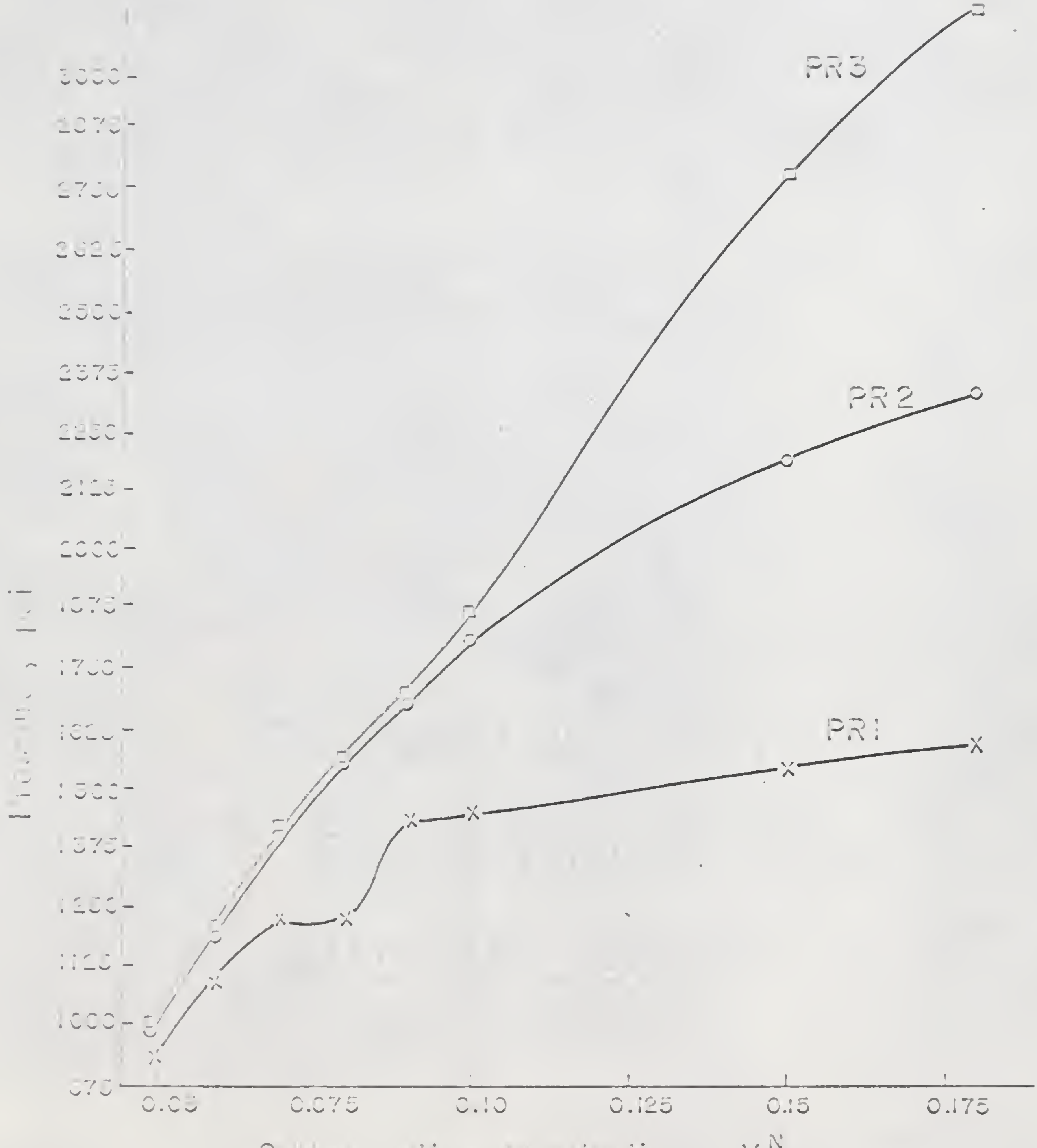


Fig. 7. Optimal operating pressure as a function of exit salt concentration for a conventional three stage system.

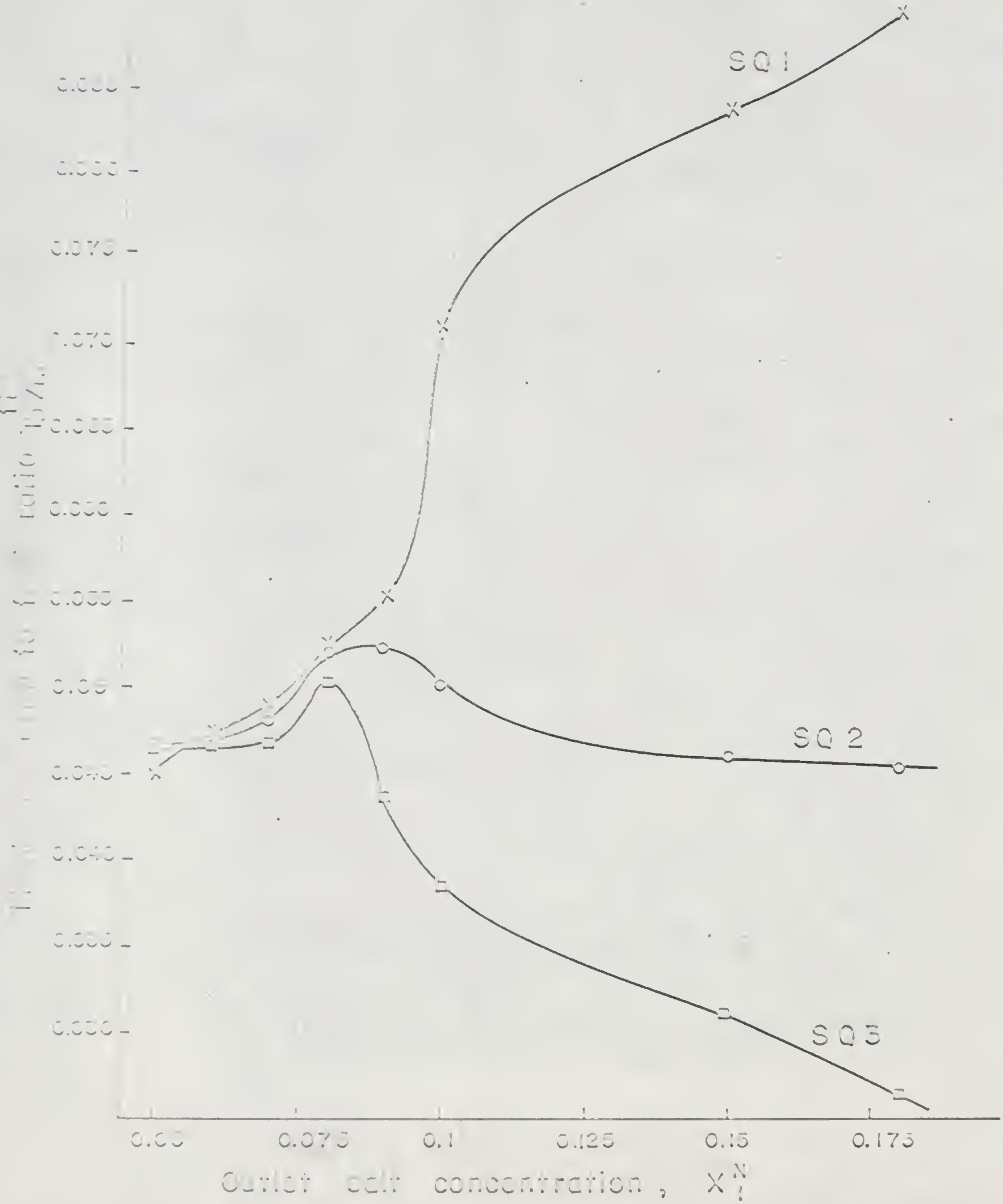


Fig. 8. Optimal membrane area to feed ratio vs exit salt concentration for a conventional three stage system.

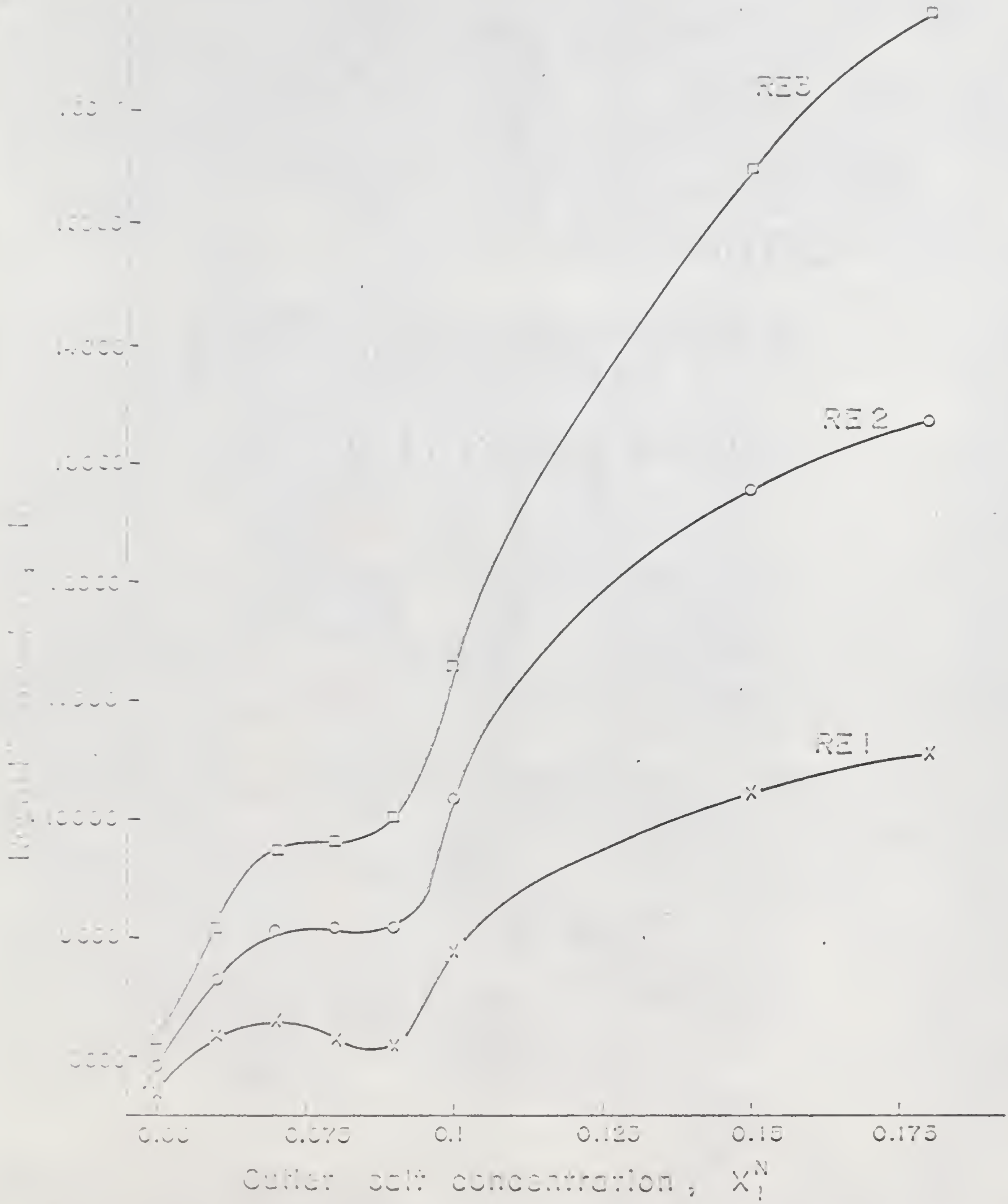


Fig. 9. Optimal Reynolds number vs exit salt concentration for a conventional three stage System.

$$\frac{S^1}{q^0} = 0.0533, \qquad \frac{S^2}{q^0} = 0.0524, \qquad \frac{S^3}{q^0} = 0.0438,$$

$$x_1^N = 0.09$$

Total cost = \$0.4397/1000 gal.

For one thousand gallons of fresh water produced per hour, the feed rate, q^0, can be calculated from the overall material balance and the corresponding membrane areas of individual stages can be evaluated. They are

$$q^0 = 13619.5 \ \ lb_m/hr.,$$

$$S^1 = 725.92 \ ft^2, \quad S^2 = 713.66 \ ft^2, \quad S^3 = 596.53 \ ft^2.$$

2. MULTISTAGE OPERATION WITH FLOW WORK EXCHANGER

(1) Formulation of Problem

The problem considered here is an extension of the problem in the preceeding section. All the performance equations are the same as those for the previous problem except for the cost functions as analyzed in the previous chapter. Therefore, in this section we only need to reformulate the performance equation for the second state variable, x_2^n. The objective function is again

$$S = x_2^N. \tag{33}$$

From Equation (2,55) the performance equations for the second state variable, x_2^n, can be expressed as follows:

$$x_2^1 = x_2^0 + A_2\,\theta_3^1\left[B_2(\theta_2^1)^{2.8} + B_3\,\theta_1^1 + B_4(\theta_1^1)^{\frac{1}{2}}\right], \qquad (34)$$

$$x_2^n = x_2^{n-1} + A_1\,y^{n-1}\,(\theta_1^n - x_3^{n-1}) + A_2\,\theta_3^n\left[B_2(\theta_2^n)^{2.8}\right.$$

$$\left. + B_3\theta_1^n + B_4(\theta_1^n)^{\frac{1}{2}}\right], \quad n = 1, 2, \ldots, N-1, \qquad (35)$$

$$x_2^N = x_2^{N-1} + A_1 y^{N-1}\,(\theta_1^N - \theta_1^{N-1}) + A_2\theta_3^N\left[B_2(\theta_2^N)^{2.8}\right.$$

$$\left. + B_3(\theta_1^N) + B_4\,(\theta_1^N)^{\frac{1}{2}}\right] + (A_3 + A_4)\theta_1^N, \qquad (36)$$

where

A_1, A_2, and A_3 are the same as defined before,

$$A_4 = B_6\,\frac{x^0}{x_1^N - x_1^0}\,. \qquad (37)$$

Similarly, the Hamiltonian functions and adjoint variables as described in Equations (12), (13), (14), and (15), and the necessary condition expressed by Equation (22) are valid for the problem.

The derivative terms relative to the second state variable, x_2^n, can be summarized as below:

$$\frac{\partial x_2^n}{\partial y_1^{n-1}} = A_1(\theta_1^n - x_3^{n-1}), \qquad n = 2, \ldots, N. \tag{38}$$

$$\frac{\partial x_2^n}{\partial x_2^{n-1}} = 1, \qquad n = 1, 2, \ldots, N. \tag{39}$$

$$\frac{\partial x_2^n}{\partial x_3^{n-1}} = -A_1\, y_1^{n-1}, \qquad n = 1, 2, \ldots, N. \tag{40}$$

$$\frac{\partial x_2^1}{\partial y_1^0} = 0, \tag{41}$$

$$\frac{\partial x_2^n}{\partial \theta_1^n} = A_1 y^{n-1} + A_2 B_3 \theta_3^n + \tfrac{1}{2} A_2 B_4 \theta_3^n \,(\theta_1^n)^{-\frac{1}{2}}, \quad n = 1, 2, \ldots, N-1 \tag{42}$$

$$\frac{\partial x_2^1}{\partial \theta_1^1} = B_1 + A_2 B_3 \theta_3^1 + \frac{1}{2} A_2\, B_4\, \theta_3^1\, (\theta_1^1)^{-\frac{1}{2}} - A_3 \tag{43}$$

$$\frac{\partial x_2^N}{\partial \theta_1^N} = A_1 y^{N-1} + A_2\, B_3\, \theta_3^N + \frac{1}{2} A_2\, B_4\, \theta_3^N (\theta_1^N)^{-\frac{1}{2}} + (A_3 + A_4) \tag{44}$$

$$\frac{\partial x_2^n}{\partial \theta_2^n} = 2.8\, B_2\, A_2\, \theta_3^n (\theta_2^n)^{1.8}, \qquad n = 1, 2, \ldots, N. \tag{45}$$

$$\frac{\partial x_2^n}{\partial \theta_3^n} = A_2 \left[B_2(\theta_2^n)^{2.8} + B_3\,\theta_1^n + B_4(\theta_1^n)^{\frac{1}{2}} \right] ,$$

$$n = 1, 2, \ldots, N. \tag{46}$$

(2) Results and Discussion

By using the same computation scheme as employed in the preceeding section, a numerical computation was performed with an IBM computer 1620. The computer program for his study is given in Appendix 5. The same numerical date were also used.

The numerical values of optimal results are listed in Table 2. In Figures 10, 11, 12, and 13, the optimal cost, optimal pressure drop, optimal Reynolds number, and optimal membrane area to feed rate ratio are plotted against the parameter, x_1^N. From these Figures we can fing the overall optimal cost and the corresponding design variables. They are

$\Delta p^1 = 1385,\qquad \Delta p^2 = 1390,\qquad \Delta p^3 = 1375,$

$Re^1 = 8070,\qquad Re^2 = 8820,\qquad Re^3 = 9470,$

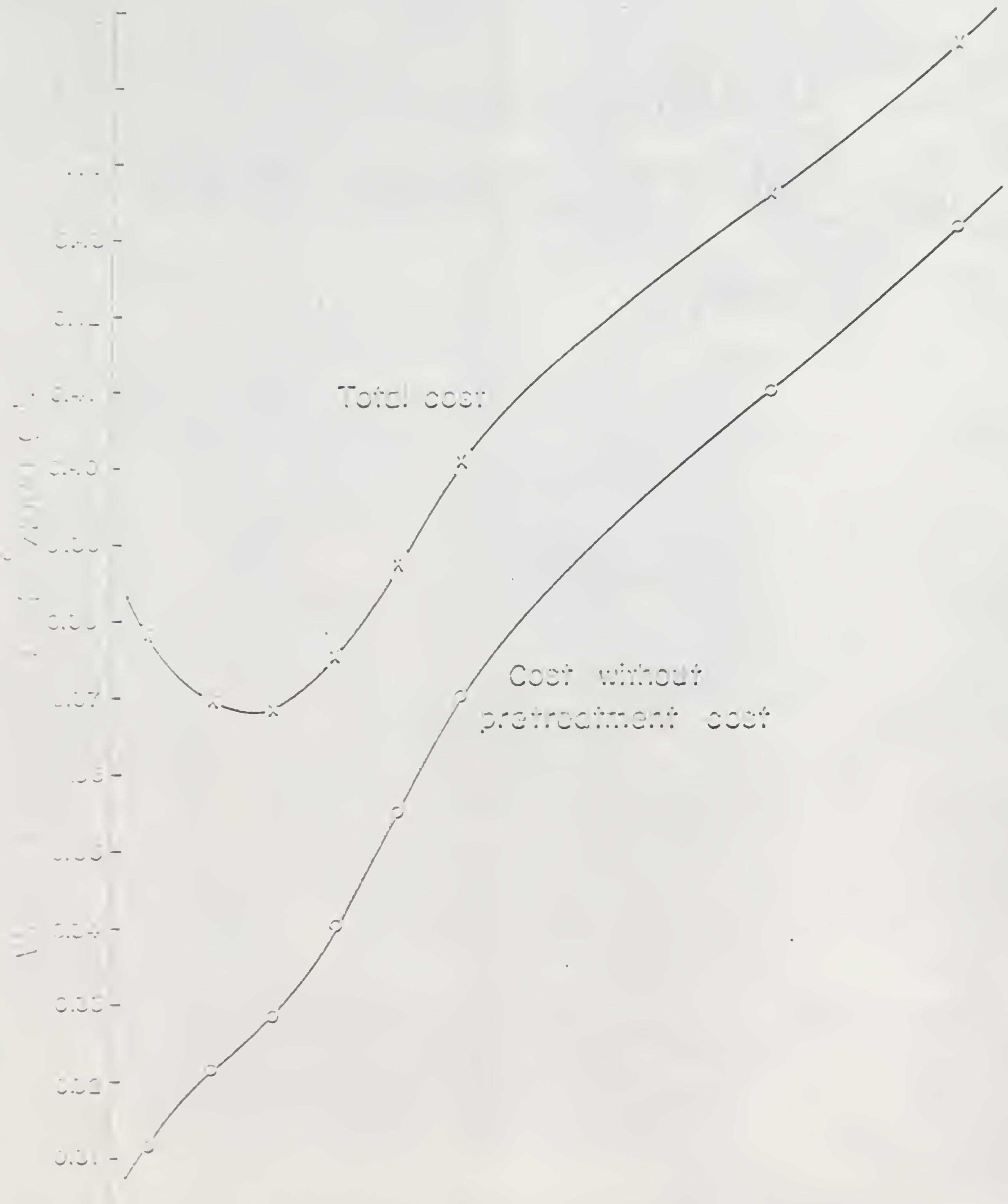
$\frac{s^1}{q^0} = 0.0465,\qquad \frac{s^2}{q^0} = 0.0465,\qquad \frac{s^3}{q^0} = 0.0465,$

$x_1^N = 0.0065,$

Total cost = \$0.3686/1000 gal.

Table 2. Optimal Conditions for a Three Stage Reverse Osmosis Process with the Use of Flow Work Exchanger for Various Outlet Salt Concentrations

Outlet Salt Concentration x_1^N, mg/L.	Pressure drop, Δp^n, psia			Reynolds Number, Re^n			Membrane area to feed ratio, $S^n/q^o \times 10^{-2}$, ft^2-hr/lb$_m$			Total Cost, Ct $/1000 gal
	1st	2nd	3rd	1st	2nd	3rd	1st	2nd	3rd	
0.05	1380.0	1370.0	1330.0	9020	9300	9440	2.35	2.35	2.35	0.3786
0.06	1210.0	1190.0	1196.3	8080	8580	9030	4.65	4.65	4.55	0.3700
0.07	1385.0	1390.0	1375.8	8070	8820	9470	4.65	4.65	4.65	0.3686
0.08	1490.0	1500.0	1507.3	8030	8920	9620	5.05	4.95	4.75	0.3760
0.09	1500.0	1670.0	1692.6	8230	9030	9950	5.40	5.10	4.30	0.3878
0.10	1390.0	1810.0	1843.1	8930	10180	11330	7.15	5.05	3.85	0.4012
0.15	1820.0	2300.0	2642.1	10850	13130	15370	7.75	3.95	2.85	0.4366
0.18	1820.0	2440.0	3137.6	10930	13550	16910	8.35	4.00	2.65	0.4569



... water production cost vs ... salt concen- ... for a three stage system with a new work ...

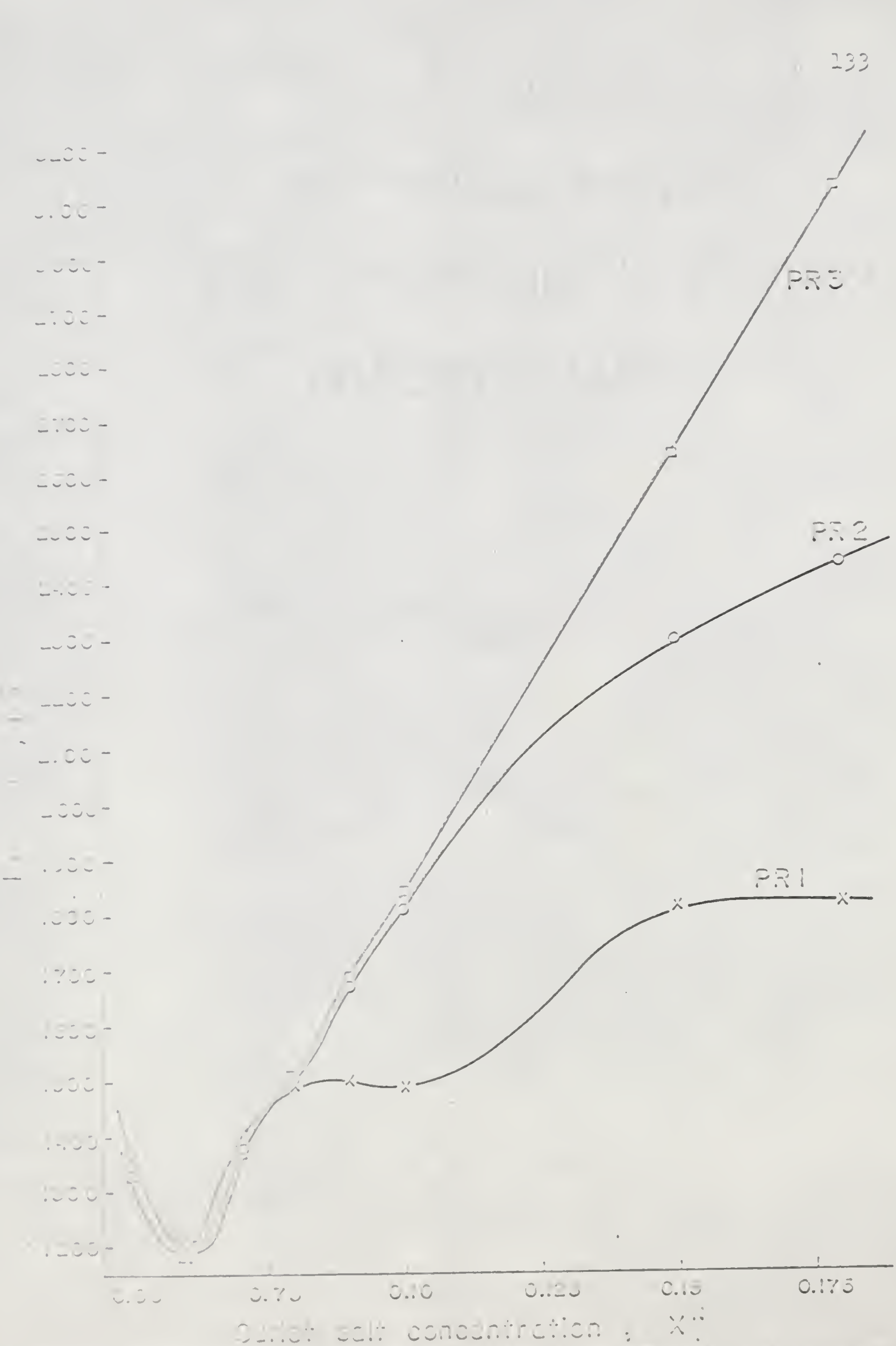
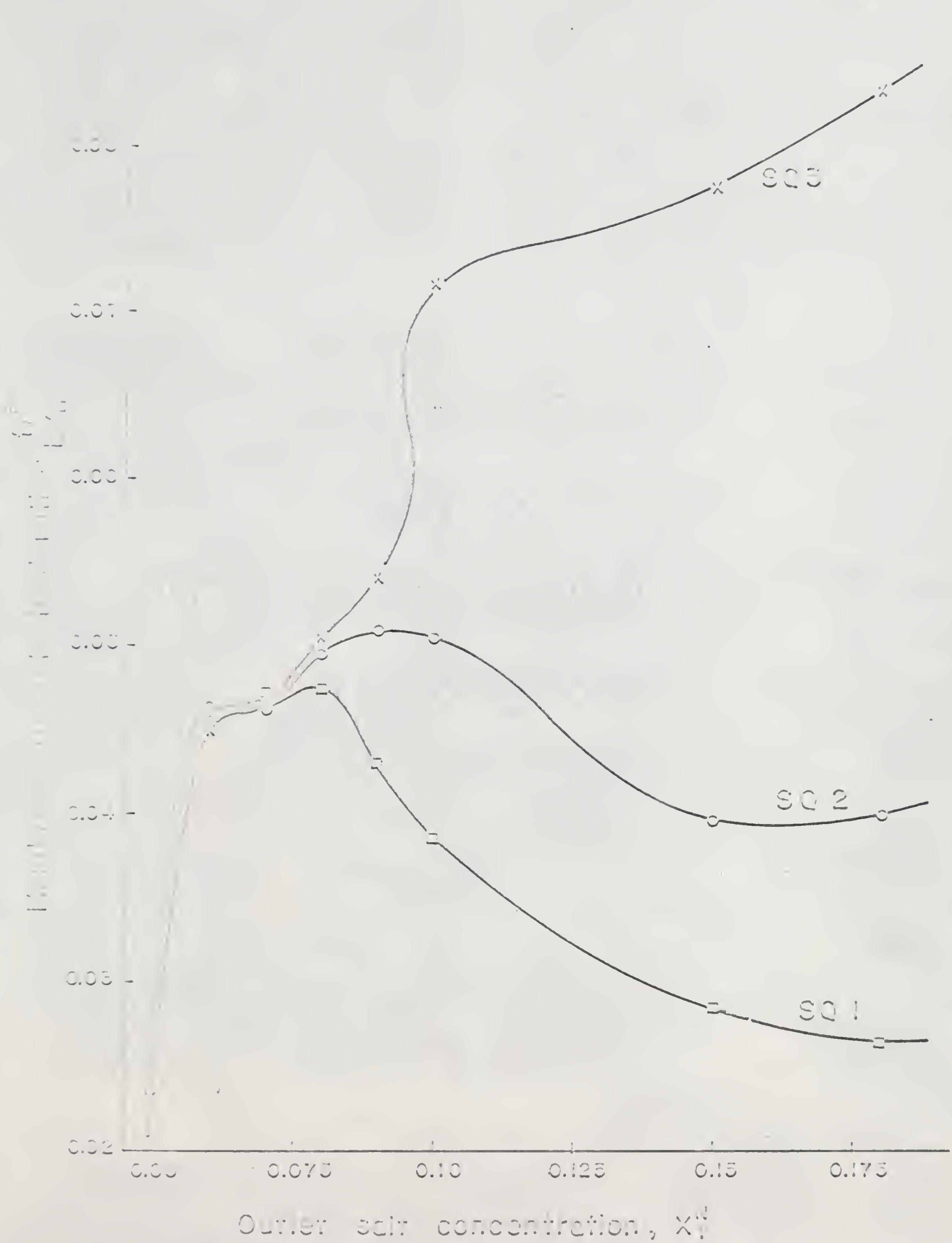


Fig. ... as a function of exit salt concentration



...2. Optimal membrane area to feed ratio vs exit salt concentration for a three stage system with a flow

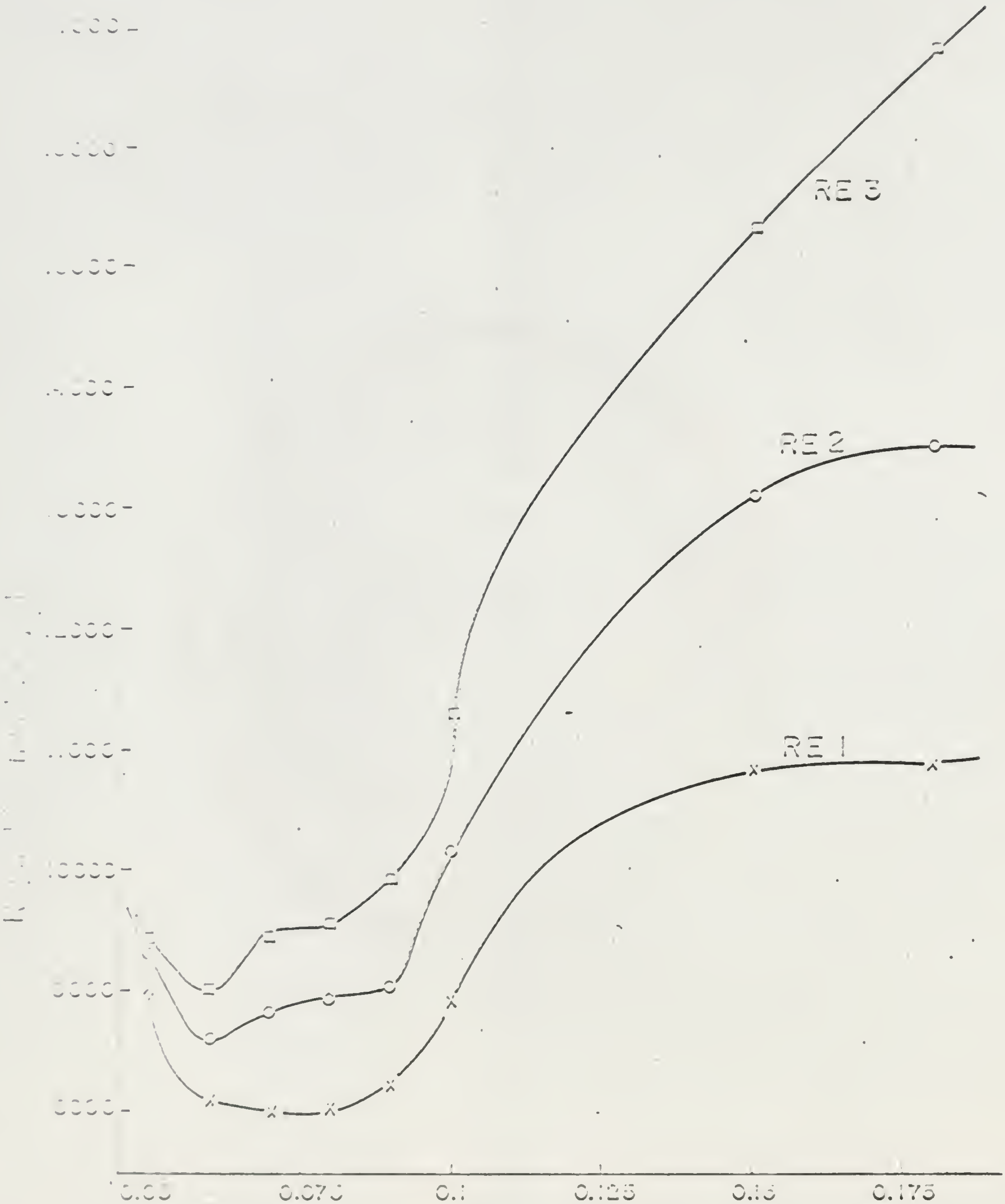


Fig. 5 Optimal Reynolds number vs exit salt concentration for a three stage system with a flow work exchanger.

For one thousand gallon of fresh water produced per hour, the feed rate, q^0, can be calculated from overall material balance and the corresponding membrane areas of individual stages can be evaluated. They are

$$q^0 = 18{,}076 \ lb_m/hr; \qquad S^1 = S^2 = S^3 = 840.53 \ ft^2.$$

By comparing the optimal results for the processes with and without the use of the flow work exchanger, the following observations can be made.

A. The use of the flow work exchanger gives rise to savings of 16 per cent in the total cost.

B. The use of the flow work exchanger substantially reduces the energy requirement.

C. The outlet salt concentration shifts from 0.09 mg/l to 0.065 mg/l .

D. Because of the reduction of the outlet concentration the feed rate increases for producing the fixed amount of fresh water when the flow work exchanger is used.

E. The use of the flow work exchanger reduces the recycle ratio at each stage.

F. The Reynolds number for flow through each stage decreases only slightly when the flow work exchanger is used. This is due to the two compensating effects given in D and E.

G. The use of the flow work exchanger increases the membrane areas required at individual stages. It is also

```
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      Z4(1)=1.
      DO 10 I=1,N
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      IF(K-N)11,12,12
   12 Z2(K)=-[illegible]
   11 [illegible]
      [illegible]
      [illegible]
      Z2(K-1)=Z2(K)*XX2(K)
      Z4(K-1)=Z4(K)
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      IF(I-N)4,9,9
    9 Z3(K-1)=-XTH(K-1)*Z2(K-1)
      GO TO 14
    4 Z1(K-1)=Z1(K)+XX1(K)*Z2(K)
   10 Z4(K-1)=Z4(K-1)
      Z2(K-2)=Z2(K-1)*XX2(K-1)
      Z1(K-2)=Z1(K-1)+Z2(K-1)*XX1(K-1)
      XTH(K)=[illegible]
      XTH(K-1)=Z1(K-1)+Z2(K-1)*XTH(K-1)
      XTH(K)=Z2(K)*XTH(K)+Z4(K)
      Z1(K)=Z1(K-1)
    1 CONTINUE
      DO 7 I=2,N
      K=2*I
      J=K-2
      L=K-3
```

OPTIMIZATION STUDIES OF ACTIVATED SLUDGE AND REVERSE OSMOSIS WATER PURIFICATION PROCESSES

by

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B. S., National Taiwan University, Taiwan 1964

AN ABSTRACT OF A MASTER'S THESIS

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MASTER OF SCIENCE

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Manhattan, Kansas

1967

ABSTRACT

The optimal designs for a step aeration activated sludge process and a reverse osmosis desalination process are carried out using a discrete version of the maximum principle together with a steepest descent search technique. Four types of systems are investigated for the overall pattern of flow, mixing, and distribution of feed for the waste treatment process. Relations are developed, which enable the feed allocation and the holding time for each stage to be chosen such that the total required volume is minimized. The use of a plug flow reactor and the allocation of feed along the system are found to be theoretically desirable for the process. Continuous feed allocation along the plug flow reactor is found to be the best system theoretically for carrying out the activated sludge waste treatment process. Relations for the reverse osmosis desalination process are developed, which enable the pressure difference across the membrane, recycle ratio, and the membrane area for each stage to be determined such that the total fresh water production cost is minimized. A flow work exchanger is employed for the desalination process in order to increase the energy recovery and thus reduce the total production cost. From the analysis, the effect of the use of the flow work exchanger in the process is found to be very significant.