A COMPARATIVE STUDY OF THE MAXIMUM PRINCIPLE AND THE MULTI-LEVEL SYSTEM THEORY AND THEIR APPLICATION

by

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INTRODUCTION

It is widely recognized that there is at present no single mathematical optimization technique superior to all other techniques in handling every type of problem. Every method has its own merits and shortcomings. Consequently, one may be suitable in solving some types of problems but becomes cumbersome in solving others. Remembering that we are dealing with the optimization of a process and that "optimizing a process" is itself a process, we would be absent-minded if we forgot to optimize what we are doing. The problem now facing us is to choose the most adequate technique to solve a specific type of problem. For some problems, the best method may be to use several techniques jointly, as is illustrated by Lee (32). In order to do so, a comparative study of all available techniques is desirable.

Since many of the processes encountered in practice, especially in the chemical industry, are so complicated that finding the optimal design and operating plans for them challenges the ability of the best engineer, a plausible approach to optimizing such formidable systems as complex chemical plants and processes is to break them down into manageable subsystems which can be optimized individually and subsequently reassemble the optimized subsystems. However, the difficulty associated with such an approach lies in taking proper account of the interactions between the subsystems, because policies which are optimal for the separate units may be disastrous for the ensemble. The multi-level system theory describes effectives ways of decomposing these large systems into component subsystems. The maximum principle is a very powerful method in solving problems of a stagewise nature. Thus we restrict our discussion to these two techniques.

In the first part of this work, we present a review of the literature on the multi-level approach of process optimization and control and a critical examination of the derivation of the multi-level optimization and control techniques.

In the second part, we discuss briefly the discrete maximum principle and extend it to a system with inequality constraints of a completely general form. We also propose two computational schemes to solve the so-called two-point boundary value problem. The comparison of the multi-level approach with the discrete maximum principle is also included in this part.

In the final part, we develop the system model and formulate equations for reverse osmosis water purification for the purpose of optimizing the process by means of the multi-level approach and/or the discrete maximum principle.

PART ONE

A STUDY OF THE THEORY OF MULTI-LEVEL SYSTEMS

CHAPTER I. INTRODUCTION

Daily activities of individuals, of gigantic enterprises, and, as a matter of fact, the activities of the whole economic system of a country have been based on a simple principle of "optimality". Observation of the similarity between the problems encountered in engineering, which include optimization and control problems, and problems which arise in the macro-economic theory should enable us to derive some mathematical techniques for the decomposition of large optimization problems.

Large-scale optimization problems have been a constant source of difficulty in both systems engineering and operations research since their inception. Roughly speaking, an optimization problem is considered "large" when the computational requirement which must be satisfied in order to find the optimal value of the manipulated variables exceeds the capacity of current computing machinery or when the quality of the performance of the system decays significantly in the time required to compute a new control solution (31). By adopting basic economic concepts, we should be able to develop simultaneously a framework for the synthesis of "organization-like" structures and at the same time use the mathematical interpretation of these "organizational structures" to develop efficient computational algorithms for large-scale optimization problems (31).

In a multi-level system, the overall system is subdivided into a number of subsystems, each of which is assigned a subobjective function (goal) and a performance equation (control).

A subsystem may represent any real or fictitious entity consisting of a finite number of stages (13).

Another level of control is assigned the object of coordinating several of the subsystems on the lower level and these in turn are coordinated by a higher level, and so on. The resulting structure, shown in Fig. 1.1, is triangular in form with the apex ultimately responsible for the achievement of the overall system object.

The conventional problem where a given system is controlled in a manner which satisfies some pre-defined objects is called a single-level optimization problem. By "single level" we mean that in general no managing or coordinating controllers are present. A characteristic of this approach is that although the overall system may consist of a complex of interconnected subsystems, the optimization technique cannot take cognizance of this fact. As a result the solution effort usually is proportional to the square or cube of the order of the problem.

A multi-level control optimization problem is one in which the structure of the subsystem is acknowledged. The conventionally phrased problem is subdivided into levels of organization, so that on the lowest level each subsystem can be optimized with respect to a subgoal. The subsystems and goals are coordinated at a third level, and so on (5).

The major advantage offered by using the multi-level approach to treat optimization problems is a reduction of dimensionality which is especially significant for large systems. In addition, the reliability of the overall system is not limited

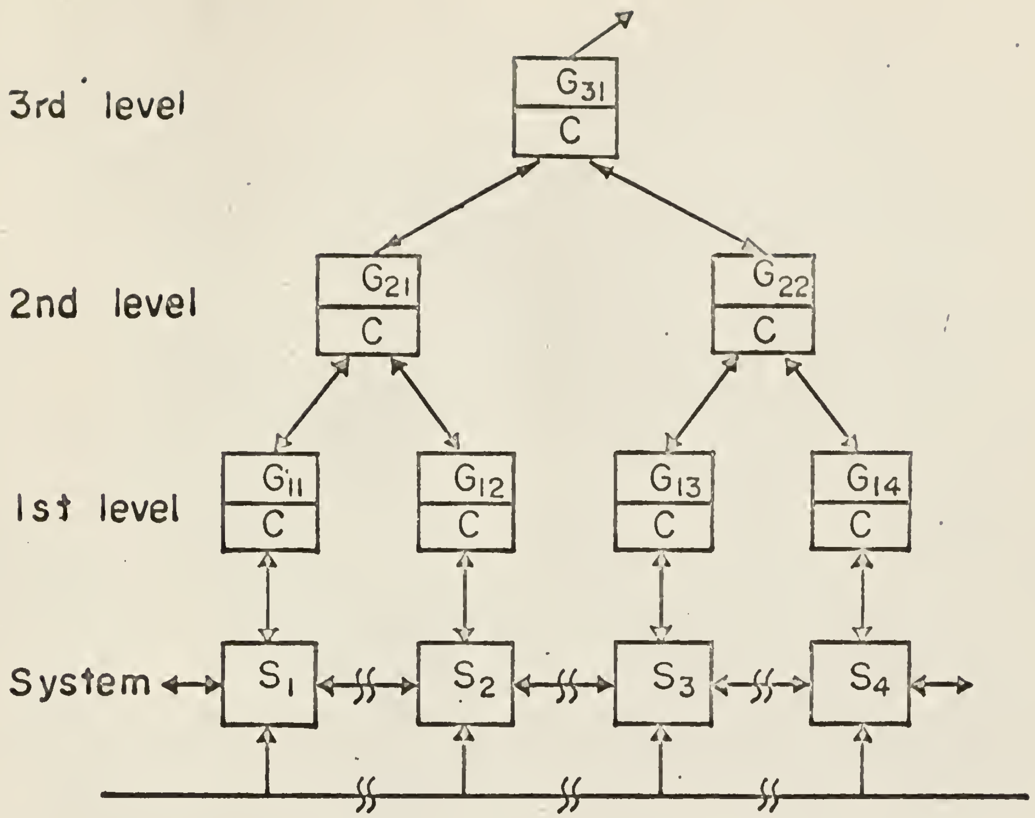

Fig. 1.1. Multi-level control structure.

S = Subsystem
G = Goal
C = Control

The arrows represent the flow of information up from lower level and the flow of control signal down from upper level.

by that of any one portion. In principle the subsystems can be arranged so that failure of one does not disrupt the performance of the other, since they are operating independently. However, the overall performance will be affected. A conventional single-level problem probably would be disrupted by failure of a subsystem since they are not operating independently. Other additional advantages are discussed in detail in references (13, 14).

The price we must pay for using the multi-level technique is the cost of coordination. Each subproblem is solved not once but many times. It is obvious that the success of multi-level techniques for an integrated system lies in the decomposition of the system.

CHAPTER II. LITERATURE SURVEY

The concept of the multi-level approach to the control of interacting systems was first introduced by Mesarovic and Eckman (1), Sprague (2), Sanders (3), and Coviello (4). The foundation of this approach is to distribute the effort for controlling a system among several subcontrollers at several levels.

Later Takahara (3) applied the multi-level systems theory to linear dynamic optimization problems in much the same way as Coviello (4). A large-scale control system which performs both the optimization function and control function is decomposed into small subsystems by neglecting the interaction between subsystems. The higher-level, goal-seeking units compensate for the neglected interaction through successive approximation of the intervention parameters as suggested by Sprague (2) and Sanders (3).

Lasdon (6) introduced a technique for the discrete process optimization by extending the concepts developed by the researchers mentioned above. He treated multi-level problems by introducing a pricing mechanism, an ideal long used by economists to achieve decentralization in economics problems. He designed a two-level structure which allows us to solve a class of discrete optimization problems by iterated solutions of subproblems. The major step in his development was the attachment of prices to the interacting variables. The problem was solved by iterating the prices. These prices were, in essence, the Lagrange multipliers of the integrated problem.

Pearson and Macko (7) extended the multi-level systems theory to a class of general dynamic optimization problems by drawing on some of the ideas presented by Lasdon (6). A set of intervention parameters to decouple the subsystems and their goals is used in their approach. For an optimal choice of the set of intervention parameters, which is determined by a higher-level controlling unit, the subgoals of each first-level subcontroller must be satisfied. This implies the satisfaction of the original system goal. Pearson (8) also considered multilevel problems from the variational point of view.

Brosilow and Lasdon (9), and Lasdon and Schoeffer (10) studied some multi-level problems using the classical Lagrange method. In this approach the second level uses the "price adjusting technique" to adjust the Lagrange parameters until a set of parameters is found such that the subproblem solutions solve the integrated problem (i.e., conventional single-level problems).

There are several papers which apply the multi-level approach to control system design. Lefkowitz (11) used the multilevel concept to break down a large overall problem into simpler subproblems as follows: (1) the process was decomposed into subprocesses, each being controlled according to a local suboptimal performance criterion, and (2) each subprocess controller was decomposed into a hierarchy of control functions which distributed the load and responsibility for satisfying the control objective.

Durbeck and Lasdon (12) presented a technique for objectively simplifying complex static optimizing control models by selecting the control model parameters and structure to maximize performance. They showed that for interconnected systems of high dimensionality the resulting parameter search may have computational difficulty. A two-level decomposition technique was used profitably to reduce this difficulty. The basic parameter search and decomposition techniques were also used in the two-time scale control approach (11), in which the assumed structure and parameters are associated directly with the control law instead of the system models.

CHAPTER III. A MULTI-LEVEL FORMULATION OF SIMPLE FEEDBACK PROCESSES (OR STATIC PROCESSES)

1. The Conventional Single-level Optimization Problem (or the Integrated Problem)

A schematical representation of the simple feedback process is shown in Fig. 1.2. The process consists of N functional subsystems interconnected in series. A portion of the output from the last subsystem is fed back to the first subsystem.

The nth subsystem produces a vector of finished products $y^{n,N+1}$ (the so-called boundary output N + 1 indicates that it goes out of the system), and a vector of intermediate or state variables x^n, which serve as inputs to the (n + 1)th subsystems. It receives both the decision variables θ^n and those variables coming from (n - 1)th subsystem x^{n-1}.

The steady-state operation of the process is described by the performance equations.

$$x^n = T^n(\theta^n, x^{n-1}) \tag{1.1}$$

$$y^{n,N+1} = V^n(\theta^n, x^{n-1}) \tag{1.2}$$

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

where x^n is an s^n-dimensional vector function, $y^{n,N+1}$ is a ν^n-dimensional vector function, and θ^n is an ω^n-dimensional vector function.

The initial feed enters the system at a rate q, whereas the feedback rate is r. The combination of the feed and the recycle stream is described by the following equation:

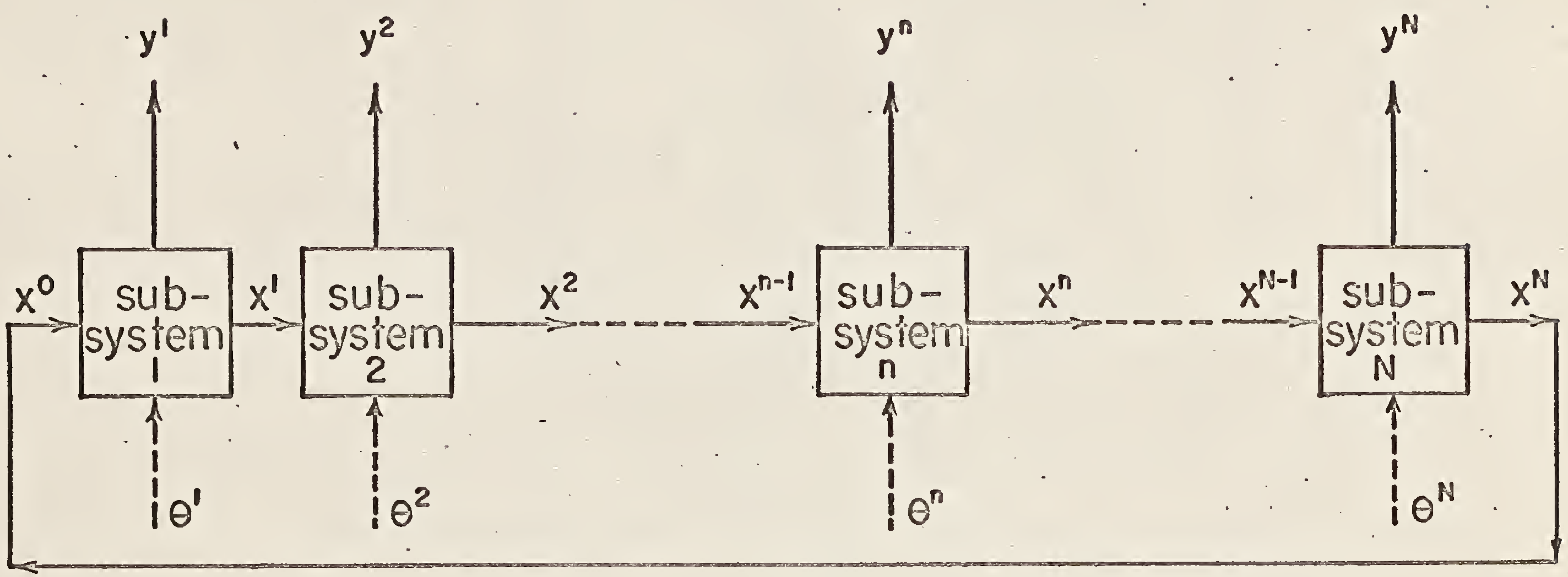

Fig. 1.2. Simple feedback process. x represents the circulated state vector; y represents the boundary output vector; θ represents the decision vector.

$$x^0 = M(x^f,\ x^N,\ q,r) \tag{1.3}$$

where M is called the mixing operator.

When the flow rates, Q and r, and feed stream conditions, x^f, are constant, equation (1.3) can be rewritten as[1]

$$x^0 = M(x^N). \tag{1.4}$$

A typical optimization problem associated with such a process, neglecting random effects, is to find a sequence of θ^n such that the objective function

$$S = \sum_{n=1}^{N} f^n(\theta^n,\ y^{n,N+1}) \tag{1.5}$$

is maximized or minimized subject to inequality constraints

$$R^n(\theta^n,\ y^{n,N+1},\ x^{n-1}) \geq 0 \tag{1.6}$$

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

where R^n is an r^n dimensional vector of function θ^n, $y^{n,N+1}$, and x^{n-1}.

The problem of finding an optimal decision vector, $\bar{\theta}^n$, which satisfies at least the necessary conditions for a maximum or minimum will be called the integrated problem (5).

We assume that all functions defined thus far are at least twice differentiable in all arguments.

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[1]Note that in this treatment components of x^f must be considered either as parameters or, if they are free, as elements of θ^1.

2. Multi-level Approach

View each subsystem as buying and selling the input x^{n-1} and output x^n from and to other subsystems (6). Associate with each x^n a vector of prices (real numbers) of the same dimension, p^n, at which these transactions take place. Let each subsystem be under the jurisdiction of a manager who views the inputs x^{n-1} as being independent as the vector θ^n is. This enables us to separate the subsystems by cutting the relations between them, that is, the performance equations, equation (1.1), are ignored. In doing this, we break up the overall problem into a number of small problems (subproblems), each of which is to be solved by a real or fictitious "first level" control unit. Thus the subproblem is also called the first-level problem. In addition we synthesize one or more "second-level control units whose function is to coordinate two or more first-level controllers.

By proceeding in this way we hope to achieve the following economics. If the process is a real one, i.e., if the imagined organizational structure can be realized, then we will enjoy the benefits of parallel operation. This is to say that several parts of the overall problem will be processed simultaneously.

If the process is imaginary, i.e., if it is simply a computational device, then we have traded the task of solving a large problem for that of solving a number of smaller ones. In either case this procedure may lead to significant computational savings.

A. The Subproblem (or the First-level Problem). Regarding p^n as parameters, the nth subproblem is for subsystem, n, described by the relations

$$y^{n,N+1} = V^n(\theta^n, x^{n-1}) \tag{1.2}$$

$$R^n(\theta^n, y^{n,N+1}, x^{n-1}) \geq 0 \tag{1.6}$$

in which a set of $\theta^n = \tilde{\theta}^n$ and $x^n = \tilde{x}^n$ that extremizes the subobjective function[1]

$$S^n = f^n(\theta^n, y^{n,N+1}) + (p^n)^T T^n(\theta^n, x^{n-1}) - (p^{n-1})^T x^{n-1} \qquad (1.7)^2$$

is found.

The subproblem solutions $\tilde{\theta}^n$ and $\tilde{x}^n$ are, of course, functions of the prices p^n. Then there exist values of p^n which are designated by $\bar{p}^n$ at which the subproblem solutions are the optimal solution of the integrated problem.

To prove the above criterion, let us define the Lagrangian for the integrated problem as

$$L = \sum_{n=1}^{N} \left\{ f^n(\theta^n, y^{n,N+1}) + (p^n)^T (T^n - x^n) + (u^n)^T R^n \right\} \tag{1.8}$$

and

$$p^0 x^0 = p^N x^N \tag{1.9}$$

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[1]Note that $\bar{\theta}^n$ denotes the solution (or optimal value) of the original integrated problem, and $\tilde{\theta}^n$ denotes the solution of the subproblems.

[2](p^n) is an s^n-dimensional vector, $(p^n)^T$ is the transpose of (p^n), and $(p^n)^T$ T (θ^n, x^{n-1}) denotes the dot product of s^n-dimensional vectors (p^n) and T^n.

where the vectors p^n, n = 1, 2, ..., N, are s^n-dimensional Lagrangian multipliers for the equality constraints, equation (1.1), and the vectors u^n, n = 1, 2, ..., N, are r^n-dimensional Kuhn and Tucker multipliers (16) for the inequality constraints, equation (1.6).

By using equation (1.9), it is seen that

$$\sum_{n=1}^{N} (p^n)^T x^n = \sum_{n=1}^{N} (p^{n-1})^T x^{n-1} . \qquad (1.10)$$

Substituting equation (1.10) into equation (1.8), the Lagrangian equation becomes

$$L = \sum_{n=1}^{N} \Big\{ f^n(\theta^n, y^n) + (p^n)^T T^n(\theta^n, x^{n-1}) - (p^{n-1})^T x^{n-1} + (u^n)^T R^n \Big\} \qquad (1.11)$$

According to Kuhn and Tucker (16), the necessary conditions for an extremum are that there exist $u^n = \bar{u}^n$ and $p^n = \bar{p}^n$ such that

$$\frac{\partial L}{\partial \theta^n} = \frac{\partial f^n}{\partial \theta^n} + (\bar{p}^n)^T \frac{\partial T^n}{\partial \theta^n} + (\bar{u}^n)^T \frac{\partial R^n}{\partial \theta^n} = 0 \qquad (1.10)$$

$$\frac{\partial L}{\partial x^{n-1}} = \frac{\partial f^n}{\partial x^{n-1}} + (\bar{p}^n)^T \frac{\partial T^n}{\partial x^{n-1}} - (\bar{p}^{n-1})^T + (\bar{u}^n)^T \frac{\partial R^n}{\partial x^{n-1}} = 0 \qquad (1.11)$$

$$\bar{u}^n \geq 0 \qquad (1.12)$$

$$(\bar{u}^n)^T R^n = 0 \qquad (1.13)$$

$$\frac{\partial L}{\partial u^n} = R^n \geq 0 \qquad (1.14)$$

$$\frac{\partial L}{\partial p^n} = x^n - T^n(\theta^n, x^{n-1}) = 0 \qquad (1.15)$$

for all n = 1, 2, ..., N.

All quantities in equations (1.12) through (1.15) are evaluated at the optimum point $\bar{\theta}^n$. But the conditions, equations (1.10) through (1.14), are equivalent to the Kuhn-Tucker conditions for the subobjective function S^n subject to $R^n \geq 0$ at the point $\left\{\bar{\theta}^n, \bar{y}^{n,N+1}, \bar{x}^n\right\}$. Thus regarding $\bar{p}^n$ as prices, we see that at these prices the subproblems satisfy the necessary conditions for an extremum at any point at which the integrated problem satisfies the same necessary conditions.

B. <u>The Second-level Problem and an Iterative Scheme (6)</u>. The fact that there exist prices p^n that decouple an integrated problem is utilized to derive an iterative procedure for optimization.

The task of finding the optimal parameters $\bar{p}^n$, n = 1, 2, ..., N, is delegated to second-level units, and the solution of the subproblems for a given set of P is the responsibility of the first-level units.[1] Note that since all the subproblems are independent, the first-level units need not communicate with each other; i.e., the constraints given by equation (1.1) can be ignored.

With the subproblem solution $\tilde{\theta}^n$ and $\tilde{x}^{n-1}$ substituted into equation (1.1), we can get the supplies from the nth subsystem, i.e., $T^n(\tilde{\theta}^n, \tilde{x}^{n-1})$. Then from the difference between the amount

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[1]Recall that $P = (p^1 : p^2 : \ldots : p^N)$.

$\tilde{x}^n$ demanded, which is determined by the n + 1th subsystem, and the amount $T^n(\tilde{\theta}^n, \tilde{x}^{n-1})$ supplied, which is determined by the nth subsystem, we can define the vector of excess demand for x^n as

$$E^n(P) = \tilde{x}^n - T^n(\tilde{\theta}^n, \tilde{x}^{n-1}) \ . \tag{1.16}$$

It is evident that if $P = \overline{P}$, $E^n(P) = 0$, $n = 1, 2, \ldots, N$. In addition, if $E^n(P) = 0$ for all n, then relations given by equations (1.10) through (1.15) are satisfied, which implies that $P = \overline{P}$. Thus we can state that $P = \overline{P}$ if and only if $E^n(P) = 0$ for all n.

The second-level adjusts the parameters P by a price adjustment rule suggested by Samuelson (17), i.e.,

$$\frac{d}{dt} p^n = E^n(P) \tag{1.17}$$

With the excess demands, $E^n(P)$, formed from the lower levels by equation (1.16) in hand, the higher level can apply a finite difference approximation to the price-adjustment rule given by equation (1.17), which will yield convergence to the optimal prices $\overline{P}$ from the feasible initial guess P_0.

Now the operation of the multi-level scheme can be described specifically. Sequentially it proceeds as follows.

1. The second-level sends to the first-level units an initial set of parameters $p^1, p^2, \ldots, p^N$.
2. Each of the first-level units optimizes its subproblem using these parameters.
3. Inputs and outputs of the first-level units are transmitted back to the second level which forms the excess

demands $E^n(P)$.

4. If these excess demands $E^n(P)$ are nonzero, the second level adjusts the parameter P by the price-adjustment rule such that the difference will be reduced and transmits these new parameters back to the first-level units.

5. The process is repeated until the excess demands are all zero, at which time the solution is optimal.

C. Convergence of the Price-adjustment Rule. It has been shown (6, 13) that if the subobjective functions S^n and the constraints R^n for all n are concave (for maximization problems) in the x^{n-1} and the θ^n for all real values of P and if at least one of these functions S^n is strictly concave, then the price-adjustment rule, equation (1.17), is asymptotically stable in the large and convergence of P to $\overline{P}$ is monotone decreasing in $\|E\|$.[1]

The stability of the price-adjustment rule is examined by Lyapunov's second method[2] (29, 30). A Lyapunov's function

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[1] $\|E\|$ is the Euclidian norm and $\|E\|^2$ is defined here as E^TE.

[2] Lyapunov's second method, Theorem II, states that if it is possible to find a function V(x) which has the following properties,

$$V(x) > 0, \quad \text{for } x \neq x_e \text{ (equilibrium point)}$$

$$V(x) = 0, \quad \text{for } x = x_e \text{ (equilibrium point)}$$

and
$$\frac{dV(x)}{dt} < 0, \text{ except for the possible case when } x = x_e,$$

$\dfrac{dV(x)}{dt} = 0$, then the system is asymptotically stable.

chosen for $\frac{dP}{dt} = E$ is

$$V(P) = \frac{1}{2}||E||^2 \qquad (1.18)$$

which satisfies

$$V(\overline{P}) = \frac{1}{2}||E(\overline{P})||^2 = 0$$

and its first-order derivative is

$$\frac{dV}{dt} = (E)^T \frac{\partial E}{\partial P} \frac{dP}{dt} . \qquad (1.19)$$

By substituting $\frac{dP}{dt} = E$ into equation (1.19),

$$\frac{dV}{dt} = (E)^T \frac{\partial E}{\partial P} E . \qquad (1.20)$$

Equation (1.20) shows that $\frac{dV}{dt}$ is the matrix of a quadratic form.

By Lyapunov's second method it is seen that asymptotic stability in the large of the price-adjustment rule, equation (1.17), requires that $\frac{dV}{dt}$ be negative definite or, equivalently, that in equation (1.20) we should have $\frac{\partial E}{\partial P}$ be negative definite for all P. We are thus led to consider in detail the elements of $\frac{\partial E}{\partial P}$. In Appendix I the negative definite of $\frac{\partial E}{\partial P}$ is proved.

D. <u>Simple Sequential Process</u>. The algorithm derived in the previous section can be reduced to a simple sequential process without feedback.

For the process without recycle, the ratio of feedback r is equal to zero, and equation (1.3) reduces to

$$x^0 = x^f \ . \qquad (1.21)$$

It is necessary to remark here that as we define x^n as an interstage variable, there is no interstage variable entering the first subsystem and leaving the last subsystem (Nth subsystem). x^0 and x^N must be equal to zero, i.e., $x^0 \equiv x^N \equiv 0$. By this treatment the relationship defined by equation (1.9) will be automatically satisfied. It is worth noting that in this treatment any initial conditions must be treated either as parameters in the first subsystem or, if they are free, as elements of θ^1. Similarly, fixed right-end conditions must be incorporated through the relations

$$y^{N,N+1} = V^N(\theta^N, x^{N-1}) \ . \qquad (1.22)$$

3. Extension

Previous sections have dealt with simple sequential processes. In this section we consider how the general nonsequential systems may be decentralized. We shall see that the same pricing adjustment scheme will suffice, but that one more parameter is now required. A full treatment of this topic is not attempted. We merely wish to indicate that an extension can be made and to demonstrate some of its major features. A special and yet very common case of recycle processes, which covers many problems considered in reference (21), is treated in more detail in section 5.

A. The Integrated Problem. The configuration of a highly nonsequential discrete system can be completely described by the equations (18)

$$x^n = f^n(y^n, \theta^n) \tag{1.23}$$

$$y^n = w^n(x^n) \tag{1.24}$$

$$y^{0n} = a^{0n} \tag{1.25}$$

$$x^{n,N+1} = V^{n,N+1}(y^n, \theta^n) \tag{1.26}$$

$$D^n(\theta^n, y^n, x^{n,N+1}) \geq 0 \tag{1.27}$$

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

where $x^n \varepsilon R^{s^n}$ are recirculated state variables. $y^n \varepsilon R^{\ell^n}$ is the total input to the nth unit from other units, and $x = (x^1, x^2, \ldots, x^N)$. $y^{0n} = a^{0n}\ R^{\ell^{0n}}$ are given constant vectors (that is, the values of the boundary inputs are preassigned). $D^n\ \varepsilon R^{d^n}$ are inequality constraints, $\theta^n \varepsilon R^{\omega^n}$ are decision variables, and $x^{n,N+1}\ \varepsilon\ R^{\ell^{n,N+1}}$ are finished products (or boundary outputs). A typical unit is shown in Fig. 1.3.

The optimization problem is to choose a set of θ^n, $n = 1, 2, \ldots, N$, such that the scalar function (the objective function)

$$S = \sum_{n=1}^{N} F^n(\theta^n, x^{n,N+1}) \tag{1.28}$$

or, by combining with equation (1.26),

$$S = \sum_{n=1}^{N} G^n(\theta^n, y^n) \tag{1.29}$$

attains its extremum values.

To derive the optimization algorithm for the problem we shall first assume that the functions $f^n(\theta^n, y^n)$, $w^n(x)$, $V^{n,N+1}(\theta^n, y^n)$, $D^n(\theta^n, y^n, x^{n,N+1})$ and $G^n(y^n, \theta^n)$ are continuous in their arguments and are at least twice differentiable in all arguments. Furthermore, we assume that a set of optimal

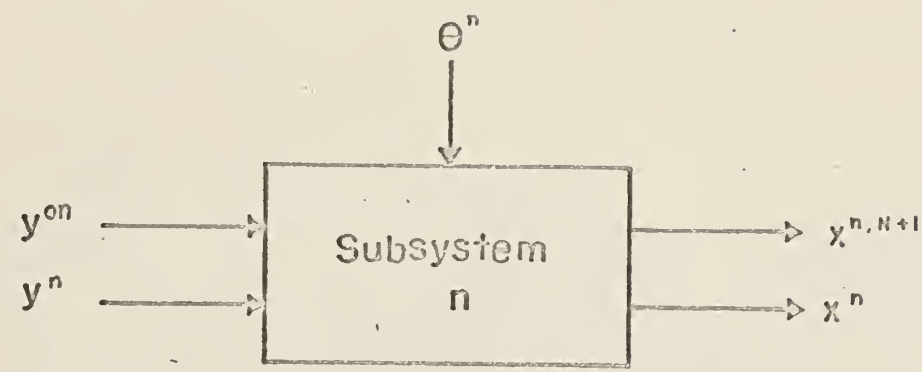

Fig. I.3. A typical subsystm of a non-sequential discrete system.

θ^n , Decision vector.
x^n : Recirculated state vector.
$x^{n,N+1}$: Boundary output vector.
y^n , Total imput vector into the n th subsystem from other subsystems.
y^{on} , Boundary input vector.

decisions denoted by $\bar{\theta}^n$, n = 1, 2, ..., N, can be found.

B. The Multi-level System Theory Approach. As previously discussed, the original overall system is subdivided into a number of subsystems each of which is assigned an optimal subproblem. An additional level of problems is assigned the goal of coordinating several of the subsystems on the lower level and these in turn are coordinated by a higher level, etc. A two-level structure is treated here.

(i) Formulation of the first-level problem

For a subsystem n, described by the equations

$$x^{n,N+1} = V^{n,N+1}(y^n, \theta^n) \tag{1.26}$$

and

$$D^n(\theta^n, y^n, x^{n,N+1}) \geq 0 \tag{1.27}$$

we are to find a set of $\tilde{\theta}^n$ and $\tilde{y}^n$, such that the subobjective function

$$S^n = G^n(\theta^n, y^n) + (p^n)^T f^n(y^n, \theta^n) - (z^n)^T y^n \tag{1.30}$$

attains its maximum for some p^n and z^n given by the second level.

(ii) Formulation of the second-level coordination problem

With the subproblem solutions $\tilde{\theta}^n$ and $\tilde{y}^n$ in hand, the second-level calculates the recirculated state variables by equation (1.23) which is

$$\tilde{x}^n = f^n(\tilde{y}^n, \tilde{\theta}^n) \tag{1.23}$$

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

With calculated $\tilde{x}^n$, a new set of the parameter z^n can be adjusted by a price-adjustment rule

$$\frac{dz^n}{dt} = y^n - w^n(\tilde{x}^n), \quad n = 1, 2, \ldots, N. \tag{1.31}$$

The parameter p^n can be computed from the new set of the parameter z^n as

$$p^n = \sum_{i=1}^{N} (z^i) \left.\frac{\partial w^i}{\partial x^n}\right|_{x=\tilde{x}} . \tag{1.32}$$

The iterative scheme is as follows:

1. The second-level assumes values for z^n and p^n and sends them to the first-level subproblems.
2. Each of the first-level subproblems optimizes its subproblem using these parameters.
3. The first-level solution, $\tilde{\theta}^n$ and $\tilde{y}^n$, is send to the second level, which forms the quantities $\tilde{x}^n$.
4. If equation (1.31) is nonzero, the second level adjusts the parameter z^n by equation (1.31) and computes the new set of parameters p^n. These new parameters are transmitted back to the first-level units.
5. The process is repeated until equation (1.31) is zero, at which time the solution is optimal.

The extension to dynamic problems is included in the next chapter.

CHAPTER IV. A MULTI-LEVEL STRUCTURE FOR LINEAR DYNAMIC OPTIMIZATION PROBLEMS

Here we are concerned with the optimization of a linear dynamic system with respect to a quadratic objective function.[1] For simplicity we assume that the problem is stationary, or time invariant in the specified time period.

1. The Integrated Problem

For a system described by a linear differential equation (5)

$$\dot{x}(t) = Ax(t) + B\theta(t) + Cd(t), \quad 0 \leq t \leq T \tag{1.32}$$

where $x(t) \varepsilon R^s$ is the state vector, $\theta(t) \varepsilon R^r$ is the decision vector, and $d(t) \varepsilon R^\ell$ are the disturbances, which are a known function of time t. A, B, and C are suitably defined constant matrices.

The boundary condition is given as

$$x(0) = a \; . \tag{1.33}$$

The problem is to find a set of $\theta(t)$, $0 \leq t \leq T$, such that the objective function

$$S = \frac{1}{2} \int_0^T \left\{ (x - y)^T Q(x - y) - \theta^T \theta \right\} dt \tag{1.34}$$

attains its minimum.

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[1]By a quadratic function we mean a homogeneous, second-degree expression in n variables of the form

$$F(x,y) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}(x_i - y_i)(x_j - y_j) \; .$$

$y \epsilon R^s$ is a reference vector, Q is constant positive symmetric matrix, and x^T denotes the transpose of x.

2. Canonical Equations

To obtain the solution to the problem, we assume that the control space of R^r of control functions $\theta(t)$ is bounded and twice continuously differentiable and that a disturbance space R^{ℓ} of disturbances d is bounded and twice continuously differentiable. We also assume that a unique set of $\overline{\theta}(t)$ and $\overline{x}(t)$, which notes S minimum, exists.

By means of the calculus of variations, we define

$$F = \frac{1}{2}\left\{(x - y)^T Q(x - y) + \theta^T\theta\right\} + z^T(Ax + B\theta + Cd - \dot{x}) \tag{1.35}$$

Then the Euler-Lagrange necessary conditions are

$$\frac{\partial}{\partial x} F - \frac{\partial}{\partial t}\left(\frac{\partial}{\partial \dot{x}} F\right) = 0 \tag{1.36}$$

and

$$\frac{\partial}{\partial \theta} F - 0 = 0 \ . \tag{1.37}$$

Or more specifically, we have

$$Q(x - y) + A^T z + \frac{dz}{dt} = 0 \tag{1.38}$$

and

$$\theta + B^T z = 0 \ . \tag{1.39}$$

At the point where t = T the transversality conditions require that for all admissible variations dx, dθ, and dt on the surface T - t = 0, we must have (5)

$$dx = \delta x + \dot{x}dt \; ; \qquad d\theta = \delta\theta \; . \tag{1.40}$$

$$\left(F - \dot{x}^T \frac{\partial}{\partial \dot{x}} F - \theta^T \frac{\partial}{\partial \theta} F\right)_{t=T} dt$$

$$+ \left(\frac{\partial}{\partial \dot{x}} F\right)^T_{t=T} dx + \left(\frac{\partial}{\partial \theta} F\right)^T_{t=T} d\theta = 0 \; . \tag{1.41}$$

Since $\delta\theta$ and δx are free differentials, the above condition becomes

$$F - \dot{x}^T \frac{\partial}{\partial \dot{x}} F - \theta^T \frac{\partial}{\partial \theta} F + \left(\frac{\partial}{\partial \dot{x}} F\right)^T \dot{x} = 0 \quad \text{at} \quad t = T \tag{1.42}$$

$$\frac{\partial}{\partial \dot{x}} F = 0 \quad \text{at} \quad t = T \tag{1.43}$$

$$\frac{\partial}{\partial \theta} F = 0 \quad \text{at} \quad t = T \tag{1.44}$$

or

$$\frac{1}{2} \left\{ (x - y)^T Q(x - y) - \theta^T\theta \right\}_{t=T} = 0 \tag{1.45}$$

$$z(T) = 0 \tag{1.46}$$

$$\theta(T) + B^T z(T) = 0 \; . \tag{1.47}$$

Combining equations (1.38), (1.39), (1.46), and (1.47) gives the following set of equations called the canonical equations.

$$\dot{x} = Ax - BB^Tz + Cd \tag{1.48}$$

$$\dot{z} = -Q(x - y) - A^Tz \tag{1.49}$$

and

$$z(T) = 0 \tag{1.50}$$

where $\theta(t) = -B^Tz(t), \quad 0 \leq t \leq T$ (1.51)

and $x(0) = a.$

Note that these canonical equations can also be derived directly from the maximum principle (18).

In order to apply the maximum principle let us introduce a new state variable $x_{s+1}(t)$.

$$x_{s+1}(t) = \frac{1}{2} \int_0^t \left\{ (x - y)^T Q(x - y) + \theta^T\theta \right\} dt \tag{1.52}$$

$$\dot{x}_{s+1} = \frac{dx_{s+1}(t)}{dt} = \frac{1}{2} (x - y)^T Q(x - y) + \theta^T\theta \tag{1.53}$$

then $\quad x_{s+1}(0) = 0 \quad$ and $\quad x_{s+1}(T) = S$. (1.54)

The Hamiltonian function will be

$$\begin{aligned} H &= z^T\dot{x} + z_{s+1}\,\dot{x}_{s+1} \\ &= z^T(Ax + B\theta + CD) + z_{s+1}\,\frac{1}{2}\left\{ (x - y)^T Q(x - y) + \theta^T\theta \right\} \end{aligned} \tag{1.55}$$

$$\frac{dz}{dt} = \dot{z} = -\frac{\partial H}{\partial x} = -A^T z - z_{s+1}\,Q(x - y) \tag{1.56}$$

$$\frac{dz_{s+1}}{dt} = \dot{z}_{s+1} = -\frac{\partial H}{\partial x_{s+1}} = 0. \tag{1.57}$$

The boundary conditions are

$$z_{s+1}(T) = 1, \qquad z(T) = 0 . \tag{1.58}$$

Substituting the boundary conditions into equation (1.57) we have

$$z_{s+1}(t) = 1, \qquad 0 \leq t \leq T . \tag{1.59}$$

The necessary condition for H to be an extremum with respect to $\theta(t)$ is

$$\frac{\partial H}{\partial \theta} = 0 \tag{1.60}$$

or

$$z^T B + \frac{1}{2}\, 2\theta = 0 . \tag{1.60a}$$

Thus we have

$$\overline{\theta}(t) = -B^T z(t) \ . \tag{1.61}$$

Substituting equation (1.59) into equation (1.56), we have

$$\dot{z} = -Q(x - y) - A^T z \ . \tag{1.62}$$

The performance equation, equation (1.32), can be derived from the Hamiltonian function as

$$\dot{x} = \frac{dx}{dt} = \frac{\partial H}{\partial z} = Ax + B\theta + Cd \ .$$

Substituting equation (1.61) into the above equation, we have

$$\dot{x} = Ax - BB^T z + Cd. \tag{1.63}$$

Thus we have shown that the canonical functions, equations (1.58), (1.61), (1.62), and (1.63) which obtained from the maximum principle, and equations (1.48) through (1.51) which obtained from the calculus of variations, are the same.

Now to apply the multi-level multi-goal structure, let us partition the performance equation and the canonical functions into $N \leq s$ subsystems.

$$\begin{pmatrix} \dot{x}^1 \\ \cdot \\ \cdot \\ \cdot \\ \dot{x}^N \end{pmatrix} = \begin{pmatrix} A_1^1 & \cdots & A_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ A_1^N & & A_N^N \end{pmatrix} \begin{pmatrix} x^1 \\ \cdot \\ \cdot \\ \cdot \\ x^N \end{pmatrix} + \begin{pmatrix} B_1^1 & \cdots & B_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ B_1^N & & B_N^N \end{pmatrix} \begin{pmatrix} \theta^1 \\ \cdot \\ \cdot \\ \cdot \\ \theta^N \end{pmatrix}$$

$$+ \begin{pmatrix} C_1^1 & \cdots & C_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ C_1^N & \cdots & C_N^N \end{pmatrix} \begin{pmatrix} d^1 \\ \cdot \\ \cdot \\ \cdot \\ d^N \end{pmatrix} \tag{1.64}$$

$$\begin{Bmatrix} \dot{z}^1 \\ \cdot \\ \cdot \\ \cdot \\ \dot{z}^N \end{Bmatrix} = - \begin{pmatrix} Q_1^1 & \cdots & Q_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ Q_1^N & \cdots & Q_N^N \end{pmatrix} \begin{Bmatrix} x^1 - y^1 \\ \cdot \quad \cdot \\ \cdot \quad \cdot \\ \cdot \quad \cdot \\ x^N - y^N \end{Bmatrix}$$

$$- \begin{pmatrix} A_1^1 & \cdots & A_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ A_1^N & & A_N^n \end{pmatrix}^T \begin{Bmatrix} z^1 \\ \cdot \\ \cdot \\ \cdot \\ z^N \end{Bmatrix} \tag{1.65}$$

$$\begin{Bmatrix} \theta^1(t) \\ \cdot \\ \cdot \\ \cdot \\ \theta^N(t) \end{Bmatrix} = - \begin{pmatrix} B_1^1 & \cdots & B_N^1 \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ B_1^N & \cdots & B_N^N \end{pmatrix}^T \begin{Bmatrix} z^1(t) \\ \cdot \\ \cdot \\ \cdot \\ z^N(t) \end{Bmatrix} \tag{1.66}$$

or

$$\dot{x}^n = A_n^n \, x^n + B_n^n \theta^n + C_n^n d^n + \sum_{\substack{i=1 \\ i \neq n}}^{N} (A_i^n \, x^i + B_i^n \theta^i + C_i^n d^i) \tag{1.67}$$

$$\dot{z}^n = -Q_n^n (x^n - y^n) - (A_n^n)^T \, z^n - \sum_{\substack{i=1 \\ i \neq n}}^{N} \left\{ Q_i^n (x^i - y^i) + (A_i^n)^T \, z^i \right\} \tag{1.68}$$

$$\theta^n = -(B_n^n)^T \, z^n - \sum_{\substack{i=1 \\ i \neq n}}^{N} (B_i^n)^T \, z^i \, . \tag{1.69}$$

The boundary conditions are

$$x^n(0) = a^n \tag{1.70}$$

$$z^n(T) = 0 \, . \tag{1.71}$$

By introducing the direct and indirect intervention variables, $\bar{s}^n$ and $\bar{\gamma}^n$, equations (1.67) and (1.68) are simplified to

$$\dot{x}^n = A_n^n x^n + B_n^n \theta^n + C_n^n d^n + E_n^n \bar{s}^n \tag{1.72}$$

$$\dot{z}^n = -Q_n^n (x^n - y^n + \bar{\gamma}^n) - (A_n^n)^T z^n \tag{1.73}$$

where

$$E_n^n \bar{s}^n = \sum_{i \neq n}^{N} (A_i^n x^i + B_i^n \bar{\theta}^i + C_i^n d^i) \tag{1.74}$$

$$Q_n^n \bar{\gamma}^n = \sum_{i \neq n}^{N} \left\{ Q_i^n (x^i - y^i) + (A_i^n)^T z^i \right\} \tag{1.75}$$

3. Multi-level Multi-goal Algorithm

The decomposition of the original integrated problem into the two-level multi-goal problems is given below.

A. <u>The First-level Problem</u>. For a subsystem n, n = 1, 2, ..., N, described by a linear differential equation

$$\dot{x}^n = A_n^n x^n + B_n^n \theta^n + C_n^n d^n + E_n^n s^n \tag{1.76}$$

we are to find a set of $\bar{\theta}^n(t)$, $0 \leq t \leq T$, such that the subobjective function

$$S^n = \frac{1}{2} \int_0^T \left\{ (x^n - y^n + \gamma^n)^T Q_n^n (x^n - y^n + \gamma^n) + (\theta^n)^T \theta^n \right\} dt \tag{1.77}$$

attains its minimum for some given direct and indirect intervention variables $s^n(t)$ and $\gamma^n(t)$ with the initial boundary condition

$$x^n(0) = a^n .$$

The solution to this problem provides time functions $x^n(t)$ and $z^n(t)$ which are then communicated to the second level.

B. The Second-level Problem. Compute a new set of $s^n(t)$ and $\gamma^n(t)$ by using

$$E_n^n s^n = \sum_{i \neq n}^{N} \left\{ A_i^n x^i - \sum_{\ell \neq n}^{N} (B_i^n)(B_\ell^i)^T z^\ell + C_i^n d^i \right\} \tag{1.78}$$

$$Q_n^n \gamma^n = \sum_{i \neq n}^{N} \left\{ Q_i^n (x^i - y^i) + (A_i^n)^T z^i \right\} \tag{1.79}$$

with the $x^n(t)$ and $z^n(t)$ computed from the first-level problems.

The operation of this organization is as follows (5):

1. Initially assume $\gamma^n = s^n = 0$. Then each subsystem is assumed to be independent and is optimized separately.
2. The subsolutions $x^n(t)$ and $z^n(t)$ are communicated to the second level from which the proposed intervention parameters, γ^n and s^n, are computed. Here $x^n(t)$ and $z^n(t)$ represent the proposed time history of resources and price levels.
3. γ^n and s^n are communicated to the subsystem and each subproblem optimized. The process is repeated until it converges within some predefined tolerance.

Now we shall prove that for any feasible intervention parameters, $\gamma^n(t)$ and $s^n(t)$, $n = 1, 2, \ldots, N$, the subproblems have unique minima. Furthermore there exists an optimal intervention $\bar{\gamma}^n(t)$ and $\bar{s}^n(t)$ such that the subproblem minima coincide with the integrated problem minimum.

To prove this let us notice that the integrated problem and subproblems are of the same class for which existence and uniqueness are guaranteed by a positive definite Q, and hence Q^n.

Comparing equations (1.76) and (1.77) with equations (1.72) and (1.73), we find that the subproblem satisfies the canonical form of the integrated problem if and only if $s^n(t) = \bar{s}^n(t)$ and $\gamma^n(t) = \bar{\gamma}^n(t)$, when $\theta^n(t) = \bar{\theta}^n(t)$.

The principal question is whether $\gamma^n(t)$ and $s^n(t)$ converge to $\bar{\gamma}^n(t)$ and $\bar{s}^n(t)$ respectively. It is shown that there exists a $T > 0$ such that the multi-level multi-goal algorithm produces a convergent sequence of intervention functions $\{\gamma^n, s^n\}$ with limits $\{\bar{\gamma}^n, \bar{s}^n\}$ for which the subproblems solve the integrated problem (5).

By introducing a set of intervention parameters, which are multipliers or prices in static systems, the general dynamic system is decomposed into a collection of decoupled small subsystems. For an optimal choice of the set of intervention parameters the satisfaction of the extremal condition of each subsystem implies the satisfaction of the extremal condition of the original system. Of course, the conditions which guarantee convergence of the intervention parameters are rather stringent when one considers nonlinear dynamic systems.

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CHAPTER V. A TWO-LEVEL OPTIMIZATION TECHNIQUE FOR DISCRETE NONSEQUENTIAL PROCESSES

Here we extend the multi-level systems theory to optimizing a class of general highly nonsequential discrete systems which was proposed by Fan, et al., (18). We shall make use of the vector-matrix notation employed by Fan, et al., in the Continuous Maximum Principle (18).

1. The Integrated Problem

The configuration of a discrete system can be described by the equations

$$x^n = f^n(y^n, \theta^n) \tag{1.80}$$

$$y^n = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} \bar{x}^{\nu} \tag{1.81}$$

$$y^{0n} = a^{0n} \tag{1.82}$$

$$y^{n,N+1} = v^{n,N+1}(y^n, \theta^n) \tag{1.83}$$

$$D^n(\theta^n, y^n, y^{n,N+1}) \geq 0 \tag{1.84}$$

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

$$\nu = 1, 2, \ldots, N$$

where $\theta^n \varepsilon T^s$ are decision variables, $x^n \varepsilon R^s$ are state variables which are equal to the recirculated output y^{nm}, m = 1, 2, ..., N, $y^n \varepsilon R^s$ is the total input to the nth unit, which is a linear combination of all the inputs, and $y^{n,N+1} \varepsilon R^s$ is the boundary output from the nth unit,[1] $y^{0n} \varepsilon R^s$ is the boundary input to the nth unit, $a^{0n} \varepsilon R^s$ is given constant vector (that is, the values of the boundary inputs are preassigned), $D^n \varepsilon R^{d^n}$ are inequality constraints, and $\Gamma^{\nu n}$ are diagonal matrices defined as

$$\Gamma^{\nu n} = \begin{bmatrix} \alpha_1^{\nu n} & 0 & 0 & \cdots & 0 \\ 0 & \alpha_2^{\nu n} & 0 & \cdots & 0 \\ 0 & 0 & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & \alpha_s^{\nu n} \end{bmatrix}, \quad n = 1, 2, \ldots, N \qquad (1.85)$$

where the diagonal elements $\alpha_k^{\nu n}$, $k = 1, 2, \ldots, s$ are non-negative scalar constants. Equation (1.81) means that the state variable of a unit itself is the output variable and that the kth component of y^n, $1 \leq k \leq s$, is a linear sum of the kth component of all y^{un}. This equation is the boundary condition for the unit function of the system, equation (1.80).

The optimization problem is to choose a set of θ^n, $n = 1, 2, \ldots, N$, such that the scalar function (the objective function)

$$S = \sum_{n=1}^{N} F^n(\theta^n, y^{n,N+1}) \qquad (1.86)$$

attains its extreme value. Substituting equation (1.83) into equation (1.86), the objective function becomes

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[1]A stream leaving the nth unit and entering the νth unit will be identified as $n\nu$th stream.

$$S = \sum_{n=1}^{N} G^n(\theta^n, y^n) \; . \tag{1.87}$$

To derive the optimization algorithm for the problem we shall first assume that the functions $f^n(y^n, \theta^n)$ and $G^n(y^n, \theta^n)$ are continuous in their arguments and that the first partial derivatives exist and are piecewise continuous in the arguments. Furthermore, we assume that a set of optimal decisions denoted by $\bar{\theta}^n$ can be found.

2. The Necessary Conditions

The Lagrangian for the overall system is

$$L = \sum_{n=1}^{N} \Big\{ G^n + (p^n)^T (f^n - x^n) + (U^n)^T R^n$$

$$+ (\lambda^n)^T \big(\Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} - y^n \big) \Big\} \tag{1.88}$$

where p^n and λ^n are the Lagrange multipliers for the equality constraints, equations (1.80) and (1.81), and U^n are the Kuhn-Tucker multipliers (16) for the inequality constraints (1.84). The U^n are constrained to be non-negative in

$$U^n \geq 0 \; . \tag{1.89}$$

We can rearrange the last term in equation (1.88) into a form which involves only the inputs and outputs of a single subsystem (or unit) n, as follows:

$$\sum_{n=1}^{N} (\lambda^n)^T \big(\Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} - y^n \big)$$

$$= \sum_{n=1}^{N} (\lambda^n)^T \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \sum_{n=1}^{N} (\lambda^n)^T \Gamma^{\nu n} x^{\nu} - \sum_{n=1}^{N} (\lambda^n)^T y^n$$

$$= \sum_{n=1}^{N} (\lambda^n)^T (\Gamma^{0n} a^{0n} - y^n) + \sum_{n=1}^{N} \sum_{\nu=1}^{N} (\lambda^{\nu})^T \Gamma^{n\nu} x^n$$

$$= \sum_{n=1}^{N} \left\{ (\lambda^n)^T (\Gamma^{0n} a^{0n} - y^n) + \sum_{\nu=1}^{N} (\lambda^{\nu})^T \Gamma^{n\nu} x^n \right\} \quad . \tag{1.90}$$

Therefore equation (1.88) can be rewritten as

$$L = \sum_{n=1}^{N} \Big\{ G^n(\theta^n, y^n) + (p^n)^T (f^n(\theta^n, y^n) - x^n)$$

$$+ (U^n)^T D^n(\theta^n, y^n, y^{n,N+1}) + (\lambda^n)^T (\Gamma^{0n} a^{0n} - y^n)$$

$$+ \sum_{\nu=1}^{N} (\lambda^{\nu})^T \Gamma^{n\nu} x^n \Big\}$$

$$= \sum_{n=1}^{N} \mathcal{L}^n(\theta^n, y^n, x^n, p^n, U^n, \lambda^1, \ldots, \lambda^N) \quad . \tag{1.91}$$

where $\mathcal{L}^n$ is the part of the Lagrangian associated with the nth subsystem.

Necessary conditions for a maximum of the objective function S subject to constraints, equations (1.80), (1.81), and (1.84), are that the Lagrangian be stationary with respect to all its arguments as given by equation (1.91). These conditions yield a set of vector equations which must be satisfied. They are:

$$\frac{\partial L}{\partial \lambda^n} = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} - y^n = 0 \tag{1.92}$$

$$\frac{\partial L}{\partial \theta^n} = \frac{\partial}{\partial \theta^n} \Big\{ G^n(\theta^n, y^n) + (p^n)^T f^n(\theta^n, y^n) + (U^n)^T D^n(\theta^n, y^n, y^{n,N+1}) \Big\} = 0 \tag{1.93}$$

$$\frac{\partial L}{\partial y^n} = \frac{\partial}{\partial y^n} \Big\{ G^n(\theta^n, y^n) + (p^n)^T f^n(\theta^n, y^n) + (U^n)^T D^n(\theta^n, y^n, y^{n,N+1}) - (\lambda^n)^T y^n \Big\} = 0 \tag{1.94}$$

$$\frac{\partial L}{\partial p^n} = f^n(\theta^n, y^n) - x^n = 0 \tag{1.95}$$

$$\frac{\partial L}{\partial x^n} = -p^n + \sum_{\nu=1}^{N} (\lambda^\nu)^T \Gamma^{n\nu} = 0 \tag{1.96}$$

$$\frac{\partial L}{\partial U^n} = D^n(\theta^n, y^n, V^{n,N+1}(\theta^n, y^n)) \geq 0 \tag{1.97}$$

$$U^n \geq 0 \tag{1.98}$$

$$(U^n)^T D^n(\theta^n, y^n, y^{n,N+1}) = 0 \tag{1.99}$$

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

It is worth noting that equations (1.97) through (1.99) are the Kuhn-Tucker multiplier conditions (16) for the inequality constraint, equation (1.84).

3. Formulation of the Multi-level System Approach

A complete decoupling of the subsystems is accomplished by either relaxing the subsystem interconnecting constraints, equation (1.81), or considering the state variables x^n as variable parameters. This isolates each subsystem from other subsystems and creates independent problems. In the second decomposition method, the solutions of subproblems always satisfy the integrated system equations. It is called the feasible decomposition method. In the first method, the overall system equations are not satisfied except at the solution of the integrated problem. This method is termed the nonfeasible method. By using these two decomposition methods, the original integrated problem can be decomposed into a two-level problem.

A. The Algorithm for a Two-level Problem by a Feasible Decomposition.[1] We have seen in equation (1.91) that the Lagrangian of the system can be broken down to a collection of ℓ^n which contains only variables associated with a single unit. It is easy to see that the necessary conditions for the Lagrangian to be stationary with respect to all its arguments are identical with the necessary conditions for ℓ^n to be stationary with respect to its arguments. This gives us a way to decompose the whole system into small subsystems or units. In fact the necessary conditions for ℓ^n to be stationary with respect to its arguments are also the necessary conditions for the subobjective function of the subsystem, n,

$$S^n = G^n(y^n, \theta^n) \tag{1.100}$$

to have an extremum in θ^n, y^n, subject to the constraints

$$x^n = f^n(y^n, \theta^n) \tag{1.80}$$

$$y^n = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} \tag{1.81}$$

$$D^n(\theta^n, y^n, y^{n,N+1}) \geq 0 \tag{1.84}$$

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[1]In this method, the following assumptions are made: (a) the vector θ^n has at least as many components as the vector x^n, and (b) the Jacobian matrix $(f^n)_{\theta^n}$ is of full rank for all θ^n and x^n.

In this formulation components of x^n are regarded as variable parameters. This suggests a two-level structure in solving the problem.

(i) The first-level problem

For a subsystem, n, described by the equations

$$x^n = f^n(y^n, \theta^n) \tag{1.80}$$

$$y^n = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} \tag{1.81}$$

$$y^{n,N+1} = V^{m,N+1}(\theta^n, y^n) \tag{1.83}$$

we are to find a set of $\tilde{\theta}^n$ with Lagrange multipliers $\tilde{p}^n$ and $\tilde{\lambda}^n$ such that the subobjective function

$$S^n = G^n(\theta^n, y^n) \tag{1.100}$$

attains its maximum for some given x^n and U^n. Here we let the inequality constraints be considered in the second level, that is, the Kuhn-Tucker multipliers U^n are delegated to the second level. This yields unconstrained and therefore simplified subproblems. This is equivalent to a modification of previous results.

(ii) The second-level coordination problem

The second-level adjusts values of x^n and U^n by using the Lagrangian differential gradient method (19), that is,

$$(x^n)_{i+1} = (x^n)_i + k \frac{\partial L}{\partial x^n} \tag{1.101}$$

$$(U^n)_{i+1} = \begin{cases} (U^n)_i - k \dfrac{\partial L}{\partial U^n}, & \text{if } U^n > 0 \\ (U^n)_i, & \text{if } U^n = 0 \end{cases} \tag{1.102}$$

and

$$D^n(\theta^n,\ y^n,\ y^{n,N+1}) \geq 0 \qquad (1.103)$$

where

$$\frac{\partial L}{\partial x^n} = -\tilde{p}^n + \sum_{\nu=1}^{N} (\tilde{\lambda}^{\nu})^T \Gamma^{n\nu} = 0 \qquad (1.96)$$

$$\frac{\partial L}{\partial U^n} = D^n(\tilde{\theta}^n,\ \tilde{y}^n,\ \tilde{y}^{n,N+1}) \geq 0 \qquad (1.97)$$

$$k > 0\ .$$

The $\tilde{p}^n$, $\tilde{\lambda}^n$, $\tilde{\theta}^n$, and $\tilde{y}^n$ are the solutions of the first-level problem, k is an arbitrary constant which is to be so chosen to drive equations (1.101) and (1.102) to convergence as quickly as possible.

A computational algorithm for this two-level structure then proceeds as follows.

1. Assume values for x^n and U^n and send to the first-level units.
2. Solve the subproblems of first-level units. This yields $\tilde{\theta}^n(x^n,\ U^n)$, $\tilde{\lambda}^n(x^n,\ U^n)$, $\tilde{p}^n(x^n,\ U^n)$, and $\tilde{y}^n(x^n)$.
3. Send the first-level solutions $\tilde{\theta}^n$, $\tilde{\lambda}^n$, $\tilde{p}^n$, and $\tilde{y}^n$ to the second level, which forms the quantities
$$\frac{\partial L}{\partial x^n} \text{ and } \frac{\partial L}{\partial U^n}\ .$$
4. If $\dfrac{\partial L}{\partial x^n} \neq 0$ and $\dfrac{\partial L}{\partial U^n} < 0$, use equations (1.101) and (1.102) to generate a new set of x^n and U^n.
5. Send new values of x^n and U^n back to the first level

and iterate from step 2 until $\frac{\partial L}{\partial x^n} = 0$ and $\frac{\partial L}{\partial U^n} > 0$. (1.104)

The above algorithm is guaranteed to converge to a global maximum of the original objective function $S(\theta^1, \theta^2, \ldots, \theta^N)$ provided $S(\theta^1, \theta^2, \ldots, \theta^N)$ and D^n are concave functions of $\theta^1, \theta^2, \ldots, \theta^N$. The algorithm converges to at least a local maximum of S provided S and D^n are locally concave. The details are given in Appendix I and reference (19).

B. <u>The Algorithm for a Two-level Problem by a Nonfeasible Decomposition</u>. Now we let the conditions

$$\frac{\partial L}{\partial \lambda^n} = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x - y^n = 0 \qquad (1.92)$$

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

be relaxed. This will separate the subsystems by cutting the links between them. Then assign arbitrary values to $\lambda^n \varepsilon R^s$ and $U^n \varepsilon R^{d^n}$. Equation (1.96) defines the P^n in terms of the assumed values of λ^n, equations (1.93) through (1.97) defines θ^n and y^n in terms of P^n, U^n, and λ^n and gives x^n in terms of θ^n and y^n. If the correct values for the λ^n have been chosen, then the values found for x^n and y^n from equations (1.93) through (1.97) will also satisfy equation (1.92). If the λ^n and U^n chosen are not correct, then equation (1.92) will not be satisfied and we must choose a different set of multipliers λ^n, U^n. This suggests a two-level structure in solving the integral problems.

(i) The first-level problem

For a subsystem n described by the equations

$$x^n = f^n(y^n, \theta^n) \qquad (1.80)$$

$$y^{n,N+1} = V^{n,N+1}(\theta^n, y^n) \tag{1.83}$$

find a set of $\tilde{\theta}^n$, $\tilde{y}^n$, $\tilde{x}^n$ such that the subobjective function

$$S_2^n = G^n(\theta^n, y^n) + (p^n)^T x^n - (\lambda^n)^T y^n \tag{1.105}$$

attains its maximum for some given λ^n and U^n.

It is evident that there exists $\lambda^n = \bar{\lambda}^n$ such that the subproblem solutions solve the integrated problems (6).

(ii) The second-level coordination problem

The second-level computes a new set of λ^n by using the price-adjustment method (6, 15).

$$(\lambda^n)_{i+1} = (\lambda^n)_i + kE^n \tag{1.106}$$

$$E^n = \frac{\partial L}{\partial \lambda^n} = \Gamma^{0n} a^{0n} + \sum_{\nu=1}^{N} \Gamma^{\nu n} x^{\nu} - y^n \tag{1.107}$$

$k > 0$

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

where k is an arbitrary constant which is to be chosen to drive E^n to zero as quickly as possible.

The adjustment of all or some of the Kuhn-Tucker multipliers, U^n, is similar to the feasible method. That is,

$$(U^n)_{i+1} = \begin{cases} (U^n)_i - k \dfrac{\partial L}{\partial U^n}, & \text{if } U^n > 0 \\ 0, & \text{if } U^n = 0 \end{cases} \tag{1.102}$$

and

$$D^n(\theta^n, y^n, y^{n,N+1}) \geq 0 . \tag{1.103}$$

A computational algorithm for this two-level structure then proceeds as follows.

1. Assume values for λ^n, U^n, $n = 1, 2, \ldots, N$, and send them to the first-level subsystems.

2. Solve the subproblems of the first-level subsystems. This yields solutions $\tilde{p}^n$, $\tilde{\theta}^n(\tilde{p}^n, \lambda^n, U^n)$, $\tilde{y}^n(\tilde{p}^n, \lambda^n, U^n)$, and $\tilde{x}^n(\tilde{\theta}^n, \tilde{y}^n)$.
3. Send the first-level solutions to the second level which forms the quantities E^n and $\frac{\partial L}{\partial U^n}$.
4. If $E^n \neq 0$ and $\frac{\partial L}{\partial U^n} < 0$, use equations (1.106) and (1.102) to generate a new set of λ^n and U^n.
5. Send new values of λ^n and U^n back to the first level and iterate from step 2, until $E^n = 0$, $\frac{\partial L}{\partial U^n} \geq 0$, for all n.

A sufficient condition for the algorithm to converge is that each subobjective function S^n be maximized for each λ^n and U^n. Proof of the convergence is given in Appendix II and reference (6, 13).

4. Discussion

A. Note that these two techniques convert an optimization problem of high dimensionality with inequality constraints into the iterated solution of a number of smaller unconstrained subproblems and simple second-level adjustment procedures. This represents a modification of the results in section 3. Since unconstrained problems are, in general, much easier to solve than problems with inequality constraints, it is desirable to delegate the Kuhn-Tucker multipliers U^n to the second level since this yields unconstrained subproblems.

B. In the nonfeasible decomposition method we can interpret the multipliers λ^n as the prices which a subsystem must pay in buying its feeds y^n from other subsystems. Similarly, p^n can be interpreted as the prices that the subsystem charges for its products which go to other subsystems. The subobjective function S_2^n is then the net profit a subsystem makes from all its transactions with other subsystems and with the outside of the system boundary with this interpretation.

x^n becomes the supply of products produced by the nth subsystem, and y^n becomes the amount which the nth subsystem demands. The function E^n is then the excess of demand over supply. The coordination algorithm represented by equation (1.106) is analogous to a competitive economy.

C. The feasible decomposition methods have been used by Mittem and Nemhauser (23), by Aris, Nemhauser, and Wilde (24), and by Nemhauser and Wilde (25) to reduce recycle problems to sequential problems which can then be treated by dynamic programming. It can be shown that feasible methods are the dual of nonfeasible methods (14). Conceptually, both feasible and nonfeasible methods have distinct economic interpretations, one as a perfectly competitive economic system, the other as a monopolistic economic scheme.

PART TWO

THE MAXIMUM PRINCIPLE AND THE MULTI-LEVEL SYSTEM THEORY

CHAPTER I. INTRODUCTION

Despite the recent profusion of work on process optimization, two areas still pose serious difficulties. The first of these encompasses problems in which the optimization is subject to inequality constraints on the process variables. Such constraints are often necessary to make the optimization meaningful, and they appear in a variety of forms. The second area deals with multidimensional processes of complex system. Any optimization is here made difficult by the implicit nature of the process model. The presence of inequality constraints further complicates matters.

In this part we shall first present an extended version of the discrete maximum principle for the optimization of simple staged processes subject to inequality constraints of a completely general form and the computational schemes to solve the so-called two-point boundary value problem. Secondly, we shall discuss the interrelationship between the discrete maximum principle and the two-level structure of the multi-level system theory. It can be shown that the adjoint variables, z^n, introduced in the discrete maximum principle will have the same function as the Lagrange multipliers (called the prices), p^n, introduced in the multi-level system theory, and that the adjoint function, i.e., $z^{n-1} = \frac{\partial H^n}{\partial x^{n-1}}$, is a necessary condition that the Lagrangian be stationary with respect to its arguments, x^{n-1}.

CHAPTER II. THE DISCRETE MAXIMUM PRINCIPLE

1. The Algorithm for the Simple Feedback Processes

The simple feedback process described previously can be represented by a set of the performance equations

$$x^n = T^n(\theta^n, x^{n-1}) \tag{2.1}$$

$$y^{n,N+1} = V^n(\theta^n, x^{n-1}) \tag{2.2}$$

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

the mixing equation

$$x^0 = M(x^N, x^f), \quad x^f = \text{given} \tag{2.3}$$

and the objective function[1]

$$S = \sum_{n=1}^{N} f^n(\theta^n, y^{n,N+1}) \ . \tag{2.4}$$

The optimization problems associated with such a process, as shown in the previous part, can be solved by the two-level system theory. It can also be shown that the same results can be obtained from the discrete maximum principle.

By introducing a new state variable x_{s+1}^n, such that

$$x_{s+1}^n = x_{s+1}^{n-1} + f^n(\theta^n, y^{n,N+1}) \tag{2.5}$$

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

with

$$x_{s+1}^0 = 0$$

---

[1]Notice that in order to obtain clarity, the inequality constraints $R^n(\theta^n, x^{n-1}, y^{n,N+1}) \geq 0$ are temporarily ignored. These are considered at the end of this section where it is shown that none of the main results are altered by their presence.

we can reduce the problem to the standard form in the discrete maximum principle.

Equations (2.1), (2.2), and (2.5) with the mixing equation, equation (2.3), completely specify an enlarged process with (s + 1) state variables and with x_{s+1}^N as its objective function, i.e.,

$$S = \sum_{i=1}^{s+1} c_i x_i^N = x_{s+1}^N \; . \tag{2.6}$$

The procedure for solving such an optimization problem by the discrete maximum principle is to introduce an (s + 1) dimensional adjoint vector z^n and a Hamiltonian function H^n satisfying (21).

$$H^n = (z^n)^T x^n \tag{2.7}$$

$$z^{n-1} = \frac{\partial H^n}{\partial x^{n-1}} \tag{2.8}$$

with the boundary conditions

$$z_i^N - \sum_{j=1}^{s} z_j^0 \frac{\partial M_j(x^N)}{\partial x_i^N} = 0 \tag{2.9}$$

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

$$i = 1, 2, \ldots, s,$$

and

$$z_{s+1}^N = 1 \tag{2.10}$$

and to determine the optimal sequence of the decision $\bar{\theta}^n$ from the conditions

$$\frac{\partial H^n}{\partial \theta^n} = 0 \tag{2.11}$$

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

or, if θ^n is constrained, the optimal decision vector $\bar{\theta}^n$ is determined either by solving equation (2.11) for θ^n when $\bar{\theta}^n$ is interior to the constrained region or by searching the boundary of the region to satisfy

$$H^n = \text{maximum} \tag{2.12}$$

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

It may be noted that the performance equations, equations (2.1) and (2.5), can be written in terms of the Hamiltonian function as

$$\frac{\partial H^n}{\partial z^n} = x^n . \tag{2.13}$$

In this problem, we have

$$z^N_{s+1} = 1 \tag{2.10}$$

and

$$z^{n-1}_{s+1} = \frac{\partial H^n}{\partial x^{n-1}_{s+1}} = z^n_{s+1} , \; n = 1, 2, \ldots, N. \tag{2.14}$$

Combining these two equations gives

$$z^n_{s+1} = 1 , \qquad n = 1, 2, \ldots, N. \tag{2.15}$$

We separate the (s + 1)th component from others, that is,[1]

$$\begin{aligned} H^n &= (\underline{z}^n)^T \, \underline{x}^n + z^n_{s+1} \, x^n_{s+1} \\ &= (\underline{z}^n)^T \, \underline{x}^n + x^{n-1}_{s+1} + f^n(\theta^n, \, y^{n,N+1}) \\ &= (\underline{z}^n)^T \, T^n(\theta^n, \, \underline{x}^{n-1}) + x^{n-1}_{s+1} + f^n(\theta^n, \, y^{n,N+1}) \end{aligned} \tag{2.16}$$

and

[1]Note that $\underline{z}^n$ and $\underline{x}^n$ are truncated vectors with s dimension.

$$\underline{z}^{n-1} = \frac{\partial H^n}{\partial \underline{x}^{n-1}} = (\underline{z}^n)^T \frac{\partial T^n(\theta^n, \underline{x}^{n-1})}{\partial \underline{x}^{n-1}} + \frac{\partial f^n}{\partial \underline{x}^{n-1}} \quad . \tag{2.17}$$

The necessary condition for an interior maximum is

$$\frac{\partial H^n}{\partial \theta^n} = (\underline{z}^n)^T \frac{\partial T^n(\theta^n, \underline{x}^{n-1})}{\partial \theta^n} + \frac{\partial f^n}{\partial \theta^n} = 0 \ . \tag{2.18}$$

The optimal solution can be obtained from solving simultaneously equations (2.1), (2.17), and (2.18) with the boundary conditions (2.9).

2. Computational Scheme

As shown in the preceding section, by the use of the maximum principle the optimization problem is reduced to that of solving a set of simultaneous equations. One of the major difficulties in such work is the solution of the so-called two-point (or split) boundary value problem, i.e., solving a set of simultaneous equations with mixed boundary conditions. It represents, in fact, the major difficulty and, although numerical analysts have given considerable attention to the two-point boundary problem, the case that arises in the study of optimization tends to be particularly difficult. One way of solving this problem is the so-called steepest ascent iteration method[1] (22).

It is recalled that according to the maximum principle,

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[1]Sometimes referred to as the "gradient method in function space" and by Merriam (26) as the "relaxation method".

θ^n is chosen to maximize the Hamiltonian H^n as a function of θ^n. The maximization requires, however, knowledge of the correct z^n. Thus there are two ways in approaching the optimal point: one starts from guessing the decision variable θ^n, and one starts from guessing the adjoint variables z^n or state variables x^n.

A. Steepest Ascent of the Hamiltonian. Suppose that the estimation of θ^n is corrected in such a direction as to increase H^n. For example, at every time the following rule might be used to proceed from the ith to the (i + 1)th approximation (22):

$$\theta^n_{(i+1)} = \theta^n_{(i)} + k \left.\frac{\partial H^n}{\partial \theta^n}\right|_{\theta^n=\theta^n_{(i)}} \tag{2.19}$$

where k is a suitable positive constant. The sequence of computations for one iteration would then be as follows:

(a) Given the ith estimate of θ^n stored in the computer (originally a guess), computations according to equation (2.1) are carried out subject to the specified initial conditions, and the resulting values of x^n are stored.

(b) Given the stored values of x^n, the adjoint functions, equation (2.17), are calculated in reverse stage number with the boundary conditions, equation (2.9). These equations are stable if the transformation equations are stable.

(c) At each step of numerical integration, as z^n becomes available, θ^n is up-dated according to rule, equation (2.19).

It has been shown (22) that for sufficiently small values of k, the sequence of computations for this iteration would converge to the optimal point, i.e., where

$$\left. \frac{\partial H^n}{\partial \theta^n} \right|_{\theta^n = \bar{\theta}^n} = 0 \ . \qquad (2.20)$$

B. Adjusting the Adjoint Variables. Let the performance equation, equation (2.1), be relaxed, which means cutting of the connection between units, and assume values of z^n, n = 1, 2, ..., N. Then, from equations (2.17) and (2.18), we can solve for θ^n and x^{n-1}. If the correct values for z^n have been chosen, the values of θ^n and x^{n-1} which are calculated from equations (2.17) and (2.18) will satisfy the performance equation, equation (2.1). If the values of z^n chosen are not correct, then the equation (2.1) will not be satisfied and we must choose a different set of values for adjoint variables, z^n, n = 1, 2, ..., N.

The adjustment of the adjoint variables depends on the amount that the performance equation (2.1) did not satisfy, i.e.,

$$z^n_{(i+1)} = z^n_{(i)} + k \left\{ x^n - T^n(\theta^n, x^{n-1}) \right\} \qquad (2.21)$$

where k is a suitable positive constant. The computational sequence for this iterative procedure is as follows:

(a) Given the ith estimate of z^n, n = 1, 2, ..., N stored in the computer (originally a guess), computations according to equations (2.17) and (2.18) are carried out subject to the boundary conditions (2.9), and the resulting values of θ^n and x^{n-1} variables are stored.

(b) With the stored values of θ^n and x^{n-1} equation (2.21) adjusts a new value of z^n.

(c) The iteration continues until equation (2.1) is satisfied.

3. Simple Sequential Process With Constraints[1]

For a process with constraints on both decision and state variables, as given in the r^n dimensional vector form

$$R^n(\theta^n, x^{n-1}, y^n) \geq 0 \tag{2.22}$$

the necessary conditions for an optimum can be obtained by combining the Kuhn and Tucker conditions (16) with the algorithm of the discrete maximum principle (21).

The Hamiltonian is defined as

$$H^n = (z^n)^T x^n + (U^n)^T R^n . \tag{2.23}$$

The necessary conditions for a saddle point in $\bar{\theta}^n$ and $\bar{u}^n$, $(\bar{u}^n \geq 0)$, that is, H^n is a maximum with respect to θ^n and a minimum with respect to u^n , are (16)

$$x^n = T^n(x^{n-1}, \theta^n) = \frac{\partial H^n}{\partial z^n} \tag{2.1}$$

$$z^{n-1} = \frac{\partial H^n}{\partial x^{n-1}} \tag{2.24}$$

$$\frac{\partial H^n}{\partial \theta^n} = 0, \quad \text{or} \quad H^n = \text{maximum} \tag{2.25}$$

$$u^n \geq 0 \tag{2.26}$$

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[1]Note that there are other treatments of this problem suggested in references (18, 27, 28).

$$(u^n)^T R^n = 0 \tag{2.27}$$

and

$$R^n \geq 0 \ , \qquad n = 1, 2, \ldots, N \tag{2.28}$$

with the boundary conditions

$$x^f = a \tag{2.29}$$

$$z_i^N = \begin{cases} 1 & \text{for } i = s + 1 \\ \sum_{j=1}^{s} z_j^0 \dfrac{\partial M_j}{\partial x_i^N} & \text{for } i = 1, 2, \ldots, s. \end{cases} \tag{2.30}$$

Note that equations (2.26) through (2.28) are the so-called Kuhn-Tucker conditions (16). There are a number of possible algorithms for solving equations (2.1) and (2.24) through (2.30).

One computational scheme suggested is a gradient search on the surface H^n, which simultaneously ascends in θ^n (the maximizing variable) and descends in u^n (the minimizing variable). The technique must, of course, take account of the restrictions, $u^n \geq 0$, and is given in the following form (19):

$$\theta^n = \theta^n + k \frac{\partial H^n}{\partial \theta^n} \tag{2.31}$$

$$u^n = u^n + k \dot{u}^n \tag{2.32}$$

where k is a suitable constant, and

$$\dot{u}_i^n = \begin{cases} 0 \ , & \text{if } u_i^n = 0 \text{ and } R_i^n > 0 \\ -R_i^n \ , & \text{otherwise} \end{cases} \tag{2.33}$$

$$i = 1, 2, \ldots, r^n.$$

The computation proceeds as follows:

(a) Choose initial values for θ^n and u^n.

(b) Find the corresponding x^n by forward solution of the performance equation, equation (2.1), with the boundary conditions, equation (2.29).

(c) Obtain the values of the adjoint variables z^n, by backward solution of equation (2.24) with the boundary conditions, equation (2.30).

(d) Evaluate $\frac{\partial H^n}{\partial \theta^n}$ and $\dot{u}^n$. If these values are nonzero, adjust θ^n and u^n by equations (2.31) and (2.32) and return to step (b).

(e) The process is repeated until $\frac{\partial H^n}{\partial \theta^n}$ and $\dot{u}^n$ are zero, at which time the solution is optimal.

The above algorithm is guaranteed (15) to converge to a global maximum of the original objective function S, provided S and R^n are concave functions of θ^n, $n = 1, 2, \ldots, N$. The algorithm converges to at least a local maximum of S provided S and R^n are locally concave.

To prove the above assertions it is necessary to prove that the gradient of the Hamiltonian without inequality constraints is the same as the gradient of the objective function S, with respect to θ^n. Such a proof can be found in references (30, 15). Once we have the desired proof, we can then fall back on the well known proofs that the Lagrangian differential gradient method converges under the above conditions (29).

Another computational scheme would be to start by assuming a set of values for z^n and u^n, $n = 1, 2, \ldots, N$. Then compute forward by using equations (2.25) and (2.26) together with the boundary conditions, equations (2.29) and (2.30), to obtain θ^n and x^n, $n = 1, 2, \ldots, N$. Using θ^n, x^n in equation (2.1), we can check if the assumed values are correct. If not, the assumed values are improved according to the following equations:

$$z^n = z^n + k \left(x^n - \frac{\partial H^n}{\partial z^u}\right) \tag{2.34}$$

$$u^n = u^n + k\,\dot{u}^n \tag{2.35}$$

where k is a suitable positive constant, and

$$\dot{u}^n = \begin{cases} 0 & \text{if } u^n = 0 \text{ and } R^n \geq 0 \\ -R^n & \text{otherwise.} \end{cases} \tag{2.36}$$

Essentially, this algorithm is the same as that described in the previous chapter. And it has been proved to converge asymptotically to the correct set of z^n and u^n, if such sub-objective function is at least locally maximized for each set of z^n (6).

CHAPTER III. THE INTERRELATIONSHIP BETWEEN THE DISCRETE MAXIMUM PRINCIPLE AND THE MULTI-LEVEL SYSTEM THEORY

We know that there exists a close relation among the maximum principle, dynamic programming, and the calculus of variations (18). In this chapter we shall show that there also exists a close relation between the maximum principle and the two-level structure of the multi-level system theory.

The multi-level system theory as presented in Part One is based on the decomposition of the Lagrangian of an integrated system. The necessary condition for the system to be extremum is that the Lagrangian be stationary with respect to all its arguments, which include the Lagrange multipliers. By decomposing the Lagrangian of the original integrated problem, the whole system is decomposed into small subsystems. Then a coordination algorithm manipulates the Lagrangian multipliers of the subproblems to the point where the solutions of the subproblems correspond to the solution of the original integrated problem. On the other hand, by introducing the adjoint variables, the discrete maximum principle decomposes the overall extremum condition into the cascaded extremum conditions. It has been shown that for a system to attain its local extremum value, it is necessary to choose a set of decision vectors such that the Hamiltonian for each unit is stationary or extremum. Therefore if we can show that the Lagrange multipliers in the multi-level system theory are the same as the adjoint variables in the maximum principle, and that the adjoint functions, i.e.,

$$z^{n-1} = \frac{\partial H^n}{\partial x^{n-1}}$$

are exactly the same as the necessary conditions that the Lagrangian be stationary with respect to its arguments, x^{n-1}, then the discrete maximum principle can be shown to be equivalent to the multi-level system theory. However, the multi-level system theory employs a price-adjustment rule for adjusting the multipliers to achieve the optimum of the original integrated problem. It also gives an economic interpretation to the subproblems resulting from the decomposition. But the discrete maximum principle neither employs any method for adjusting the adjoint variables to achieve the optimum of the problem nor makes use of any economic interpretation to the decomposition.

In proving that the adjoint variables and the Lagrange multipliers are the same, considering only the simple feedback discrete cases, there will be little loss of generality. The simple feedback discrete cases have been treated in detail in Chapter III, Part One, by the multi-level system theory and by the maximum principle in section 1, Chapter II, Part Two.

By comparing the necessary conditions derived from the discrete maximum principle, equations (2.24) through (2.29), with those derived from the multi-level system theory, equations (1.10) through (1.15) in Part One, we see that the Lagrange multipliers, (or the prices of x^n), p^n, in the multi-level system theory are actually the adjoint variables z^n in the discrete maximum principle, and that the adjoint function, equation (2.24), of the maximum principle is actually a necessary condition that the Lagrangian be stationary with respect to its arguments x^{n-1}, equation (1.11) in Part One.

By comparing the computational schemes, it is easy to recognize that the price-adjustment rule, equation (1.17) in Part One, used in the second-level problem of the multi-level theory is exactly the same as the rule for adjusting the adjoint variables, equation (2.21), suggested in the preceding sections.

In the feasible decomposition method of the multi-level system theory, derived in section 3, Chapter V, Part One, it is assumed that the decision vector θ^n has at least as many components as the state vector x^n and the Jacobian matrix $(f^n)_{\theta^n}$ is of full rank of all θ^n and x^n. It is easy to recognize that if the components of vector θ^n and x^n are exactly the same, the feasible decomposition method and the steepest ascent of the Hamiltonian method suggested in the preceding section will be identical. However, if the components of the decision vector θ^n are fewer than the components of the state vector x^n, then the feasible decomposition method fails. This appears to be the weak point of the feasible decomposition method. On the other hand, if the components of the decision vector θ^n are more numerous than the components of the state vector x^n, the steepest ascent of the Hamiltonian method fails. This means that the system will be overdetermined when all the decision variables are specified, that is, the number of the decision variables will be greater than the number of the independent variables. In this case we should use the feasible decomposition method. Or, if the state variables are interchanged with the decision variables, the method of the steepest ascent in the Hamiltonian space can be used.

So far we have compared only the two-level structure of the multi-level system theory with the discrete maximum principle for the simple feedback process. It is plausible to extend this comparison and identification to the multi-level structure, which is more complex than the two-level structure. However, such an extension appears to be, if not impossible, extremely difficult. And the use of the multi-level system theory alone to optimize the complex multi-level structure also appears to be very tedious if compared with the use of the maximum principle.

Although the multi-level system theory and the discrete maximum principle can be proved to be mathematically equivalent, the way of approach to an optimization problem according to each method is quite different. By means of the multi-level system theory, we can decompose the whole integrated system into subsystems with smaller dimensions. The subsystems then may be solved by any of the existing optimization techniques. Thus it is plausible to construct, by combining the multi-level approach with the discrete maximum principle, a powerful method for optimizing the highly dimensional complex system. This should be an area for future work.

PART THREE

PROCESS ANALYSIS AND DESIGN OF A SEQUENTIAL REVERSE-OSMOSIS WATER PURIFICATION SYSTEM

CHAPTER I. INTRODUCTION

The reverse-osmosis water purification process consists of raising the pressure of an aqueous solution to a pressure above its osmotic pressure and bringing it into contact with a selective membrane which is much more permeable to water than to the impurities (solutes).

The use of reverse osmosis for water purification is being considered for saline water, brackish water, and process waste water. The process is also being considered for water purification in remote areas where only small quantities of water are needed. The process analysis and design study in this paper are primarily intended for those applications where saline and brackish waters are to be purified.

Because of its simplicity and low energy requirements (the water undergoes no phase change and temperature changes are small), reverse osmosis has been drawing widespread favorable attention as a purification technique. It is now well established that synthetic osmotic membranes, made of cellulose acetate, formamide, and acetone, can be produced which are highly permeable to water and sufficiently impermeable to dissolved salts. Although the reproducibility and durability of these membranes are still in doubt, the results obtained to date are sufficiently encouraging to warrant a closer look at the possible economics of reverse osmosis as a water-desalting process.

This study is an attempt to investigate the reverse-osmosis process in order to find ways in which the design can be improved.

A boundary layer flow model of the reverse-osmosis unit is devised. It is based on boundary-layer theory and one-dimensional diffusion theory. A set of system equations or a system model which relates the flow rate, energy requirement, and cost is then formulated. It is often desirable to formulate a model which simulates the behavior of the process. This model may then be used to find the optimum design and operating conditions of the system. The design of a system of reverse osmosis units connected in simple sequence is investigated in this study.

The proposed sequential process is described and its advantages are qualitatively discussed in section 2. In section 3 a boundary-layer flow model is derived and the process based on this model is analyzed for calculating the flow rate of fresh water through the membrane. In section 4, the power requirement for the process is determined and the cost function is derived. A conceptual design of the process is given in section 5.

CHAPTER II. DESCRIPTION OF PROCESS

The simplicity of the reverse-osmosis process is apparent upon inspection of a flowsheet of the Aerojet pilot plant (33). 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. The minimum energy requirement in an ideal reverse-osmosis process would be achieved by applying a differential pressure, ΔP, across the membrane. In other words, the pressure difference should be only infinitesimally greater than the osmotic pressure of the brine solution. The concentration of the brine solution should be allowed to increase only infinitesimally in the process. A blowdown turbine can be used to recover the energy of the high pressure reject brine solution. However, in the real process there is an energy loss due to increasing the pressure of the main brine solution above the osmotic pressure and then rejecting it to atmospheric pressure. Therefore there is a minimum energy requirement for the process, which is different from that for the ideal process. Furthermore, the fresh water flux through the osmotic membrane is a function of the pressure difference across it, which is the so-called driving force. To minimize the capital cost of the separating unit requires separating pressures substantially above the osmotic pressure of the most concentrated brine in the system. Thus an economic balance between energy and capital costs must be achieved by the proper selection of operating pressure and reject-brine concentration.

As we have just stated, the pumping work is related to the osmotic pressure of the brine solution. The energy consumption is proportional to the pressure required in each stage. The higher the osmotic pressure in the separator units, the greater the energy consumption. The osmotic pressure of sea water containing 35,000 p.p.m. (i.e., 3.5 wt. per cent) total salts is approximately 24 atm. (47). In diluted sea water it is roughly proportional to the salt concentration. As fresh water is removed from the brine solution the salt concentration at the membrane boundary becomes higher than that of the bulk solution. Accordingly the effective osmotic pressure, which is the osmotic of the solution at the membrane surface, increases. This effect of salt build-up at the membrane surface is significant with present-day membranes. It may become an increasingly more important problem as better membranes are developed. This boundary-layer effect will be discussed in more detail later. To reduce this boundary-layer effect, the concentrated brine solution in the boundary layer should be mixed with the main stream at frequent intervals or the bulk solution flow rate should be increased in order to reduce the thickness of the boundary layer. This may be accomplished by using a recycle flow to keep the flow in a turbulent condition.

In an attempt to optimize the design of a reverse-osmosis process, Lonsdale, et al. (34) considered a simple one-separator unit operation. The discharge salt solution in their best result contains nearly 6 wt per cent of salt. To reduce the boundary-layer effect, they proposed the use of a recycle flow. However, from the viewpoint of thermodynamics, it is unwise to mix 6 wt per cent solution with 3.5 wt per cent (average) sea water. Thus we propose a multi-stage sequential system as shown in Fig. 1.

Since the osmotic pressure is proportional to the brine concentration in diluted brine solutions, it is advantageous to use a low pressure in the first stage where the concentration

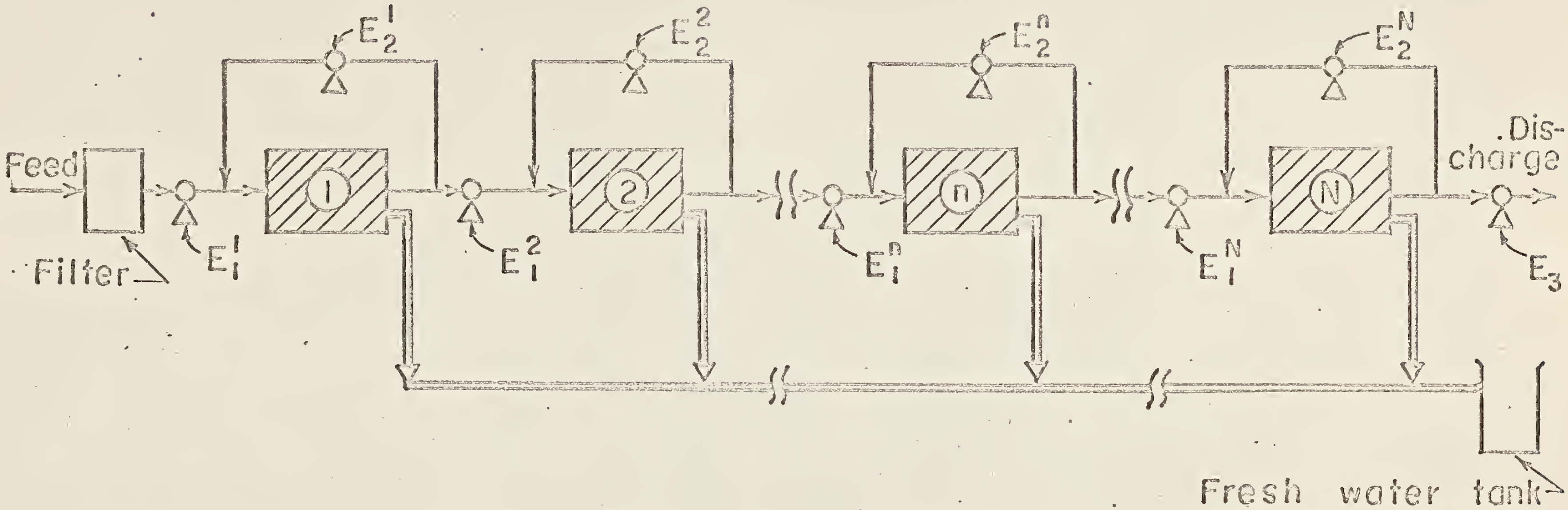

Fig. 1. Schematic diagram of a sequential reverse osmosis water purification process.

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 blowdown turbine at end of the process

$\longrightarrow$: brine solution

$\Longrightarrow$: fresh water product

 : the membrane separator unit at n-th stage

of salt is the lowest. The brine concentration increases as the brine solution progresses through the plant. Therefore we shall use a stepwise increase in pressure from stage to stage, that is, the plant will operate at as nearly an ideal reverse-osmosis process as possible. Thus we insert a high pressure pump between stages, which is used to increase the pressure in the process from one stage to the next.

Instead of mixing the high concentration output with the relatively lower concentration inlet, we propose to use recycle flow at each stage. Thus we insert a bring circulation pump to recycle the flow in each stage.

For each stage, we use a conceptual shell-and-tube design arrangement which clearly gives a lower capital cost per unit membrane area than does the plate-and-frame configuration.

CHAPTER III. ANALYSIS OF PROCESS

1. Boundary-layer Flow Model

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 the 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 through the membrane is zero. This means that the effective osmotic pressure is greater than that of the bulk solution. The situation near the membrane boundary is shown in Fig. 2. If we insert a circulation pump at each stage, it is possible to make the flow in the tubes be in the region of fully developed turbulent flow, that is, the bulk solution flowing parallel to the osmotic membrane surface is well mixed, and the existence of concentration and velocity gradients is mainly confined to the laminar boundary layer.

In the absence of chemical reaction the ratio between the concentration boundary-layer thickness, δ_c, and the momentum transport boundary-layer thickness, δ, is shown by Bird, et al. (35) to be a constant which is dependent only on the value of the Schmidt number, i.e.,

$$\frac{\delta_c}{\delta} = Sc^{-1/3}$$

or

$$\delta_c = \delta \cdot Sc^{-1/3} \tag{1}$$

where Sc is the Schmidt number which is equal to the kinematic viscosity , divided by the diffusion coefficient for the solution, D_a, or

$$Sc = \frac{\nu}{D_a} . \tag{2}$$

The thickness of the laminar sublayer for turbulent flow through pipes is given in Schlichting (4) to be equal to

$$\delta \approx 5 \frac{\nu}{v_*} \tag{3}$$

where ν is the kinematic viscosity $(\frac{\text{sq cm}}{\text{sec}})$, and v_* is the friction velocity defined as

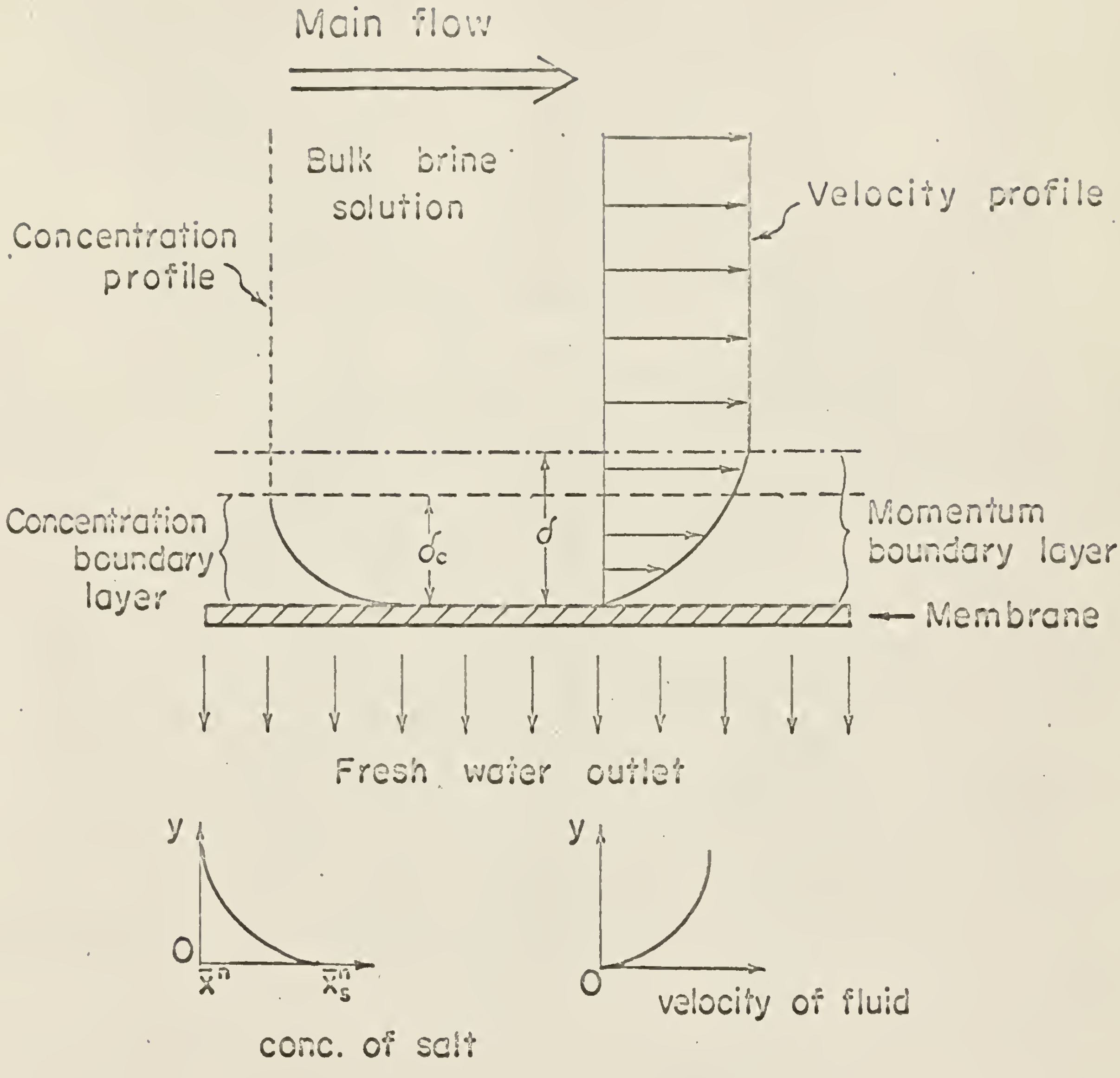

Fig. 2. Velocity and salt concentration gradients in boundary layer adjacent to a membrane.

$$v_* = \sqrt{\tau_0 / \rho} \tag{4}$$

in which τ_0 is the shearing stress at the wall. v_* is a measure of the intensity of turbulent eddying and of the transfer of momentum due to these fluctuations. For turbulent flow through pipes, the shearing stress, τ_0, can be calculated from the following equation (4):

$$\tau_0 = 0.0225\, \rho U^{7/4} \left(\frac{\nu}{R}\right)^{1/4} \tag{5}$$

where ρ is the density of the fluid and U the maximum velocity which is proportional to the mean velocity $\hat{u}$. The ratio $\frac{\hat{u}}{U}$ equals 0.8 for turbulent flow through pipes. R is the radius of a pipe and d = 2R denotes the diameter of the pipe. Introducing d into equation (5) and then substituting equations (4) and (5) into equation (3) yields

$$\delta = \frac{5\,\nu}{\sqrt{\frac{\tau_0}{\rho}}} = \frac{5\nu}{\sqrt{0.0225\; U^{7/4} \left(\frac{\nu}{d\;2}\right)^{1/4}}}$$

$$= \frac{5}{\sqrt{0.0225}\;.\;2^{1/8}\;.\;\left(\frac{\hat{u}}{0.8}\right)^{7/8}\;.\;d^{-1/8}\;.\;\nu^{(1/8-1)}}$$

$$= \frac{5\cdot(0.8)^{7/8}\, d}{0.15\cdot 1.09\; \hat{u}^{7/8}\, d^{7/8}\, \nu^{-7/8}}$$

$$= \frac{33.3\cdot(0.824)\; d}{1.09\;\left(\frac{\hat{u}d}{\nu}\right)^{7/8}}$$

$$= \frac{25.2\;d}{\left(\frac{\hat{u}d}{\mu}\right)^{7/8}} = \frac{25.2\;d}{Re^{7/8}} \tag{6}$$

where $Re = \frac{\hat{u}d}{\nu} = \frac{\hat{u}d}{\mu}$ is the Reynolds number. Substituting equation (6) into equation (1), we obtain

$$\delta_c = \frac{25.2\ d}{Sc^{1/3}\ Re^{7/8}} \ . \tag{7}$$

In a sequence of stages the concentration and velocity differ from stage to stage. If the viscosity, density, and diffusivity are assumed to be constant, and the diameter of the tubes is assumed to be the same in each stage, then the velocity will change at each stage. Thus the Reynolds number will be different in each stage. The concentration boundary-layer thickness at the nth stage then becomes

$$\delta_c^n = \frac{25.2\ d}{Sc^{1/3}\ (Re^n)^{7/8}} \qquad (7a)^1$$

From equation (7) it can be recognized that the larger Reynolds number which can be achieved by increasing the circulation rate reduces the boundary-layer thickness. Thus the increase in osmotic pressure arising because of the boundary layer will undoubtedly have to be controlled by providing adequate circulation rates through the tubes. We have assumed that the system is isothermal and that there is no precipitation of salt on the membrane surface. The experimental result of Merten (37) suggests that alternative procedures may be devised to control salt precipitation. The effects of circulation on flow through an osmotic carrier have been experimentally observed by

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[1]Note that the superscript number n indicates the stage number. Exponents, where required, will be written outside of parentheses or brackets.

Merten (37). His results are in good agreement with equation (7).

2. Simple Sequential Multi-stage System

The proposed sequential reverse-osmosis water desalination system shown in Fig. 1 is of the form of a simple sequential multi-stage model (39) as shown in Fig. 3. Each stage, except the last stage, includes a membrane separator unit, a recycle pump, and a high pressure pump between stages. Figure 4 gives a schematic representation of the nth stage. The last stage, stage N, includes a blowdown turbine in its outlet.

Let us now define the following symbols:

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

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

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

W_f = the total mass flow rate of fresh water produced from the whole system, ($\frac{lb_m}{hr}$), that is,

$$W_f = \sum_{n=1}^{N} W^n \tag{8}$$

N = the total number of stages in the sequence of the process.

Here we assume that the salt concentration of fresh water produced is negligible. We also assume that the recirculation rate

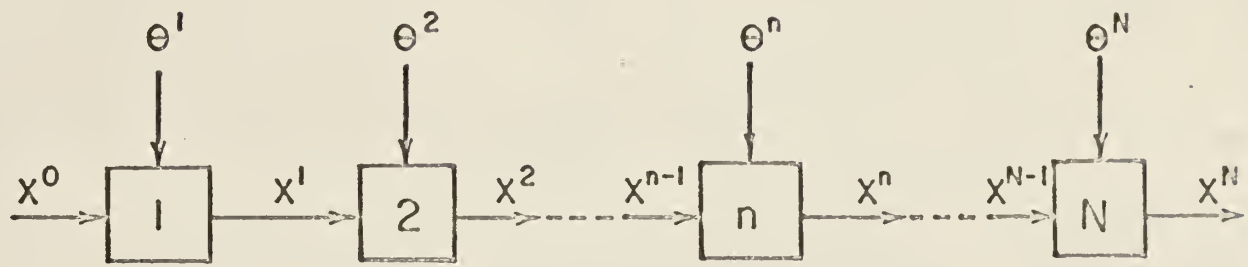

Fig. 3. Simple sequential N-stage model.

Where x represents the state vector.

θ represents the decision vector.

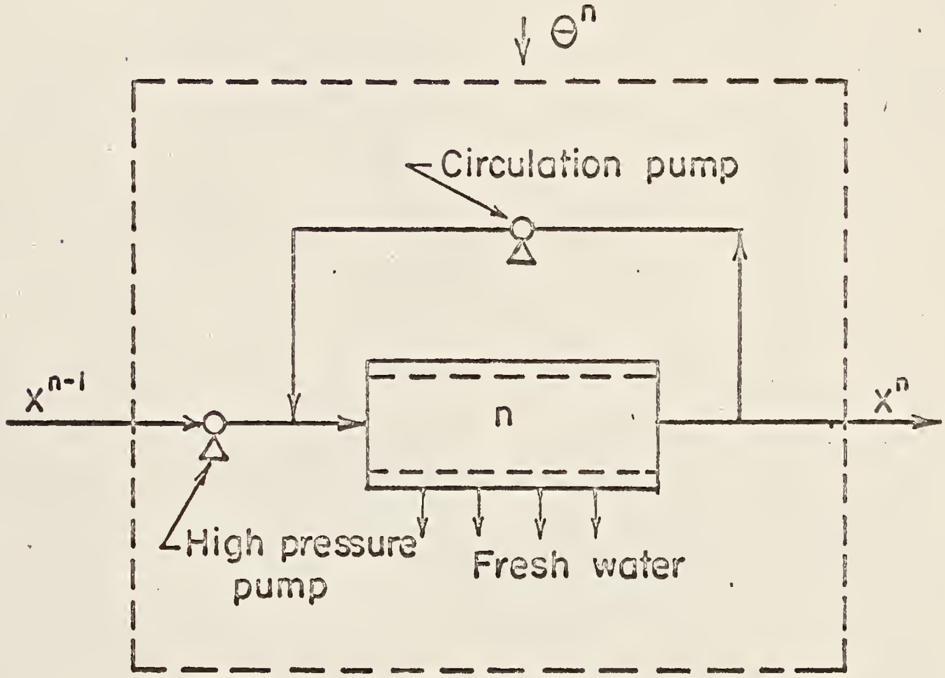

Fig. 4. The representation of a single stage.

Where x represents the state vector.
Θ represents the decision vector.

is sufficiently high with W^n. Therefore we may also assume that the salt concentration in the bulk solution is constant, that is, $\hat{x}^n = \hat{x}^n$, where x^n is the salt concentration of the brine stream leaving stage n.

Then the total material balance for the process as a whole is

$$q^0 = q^N + W_f . \tag{9}$$

The salt material balance for each stage is

$$q^0 x^0 = q^1 x^1 = \ldots = q^n x^n = q^n x^n . \tag{10}$$

3. The Volumetric Flow Rate of Fresh Water Produced at the nth Stage, F^n

The volumetric flux of water, F^n, through a membrane of constant permeability has been reported by Merten (37) as

$$F^n = K(\Delta P^n - \pi_S^n) \left(\frac{ft^3}{ft^2 - hr}\right) \tag{11}$$

where K = the membrane constant $\left(\frac{ft^3}{ft^2 - hr - psi}\right)$

ΔP^n = the pressure difference across the membrane of the nth stage (psi)

π_S^n = the osmotic pressure of the brine solution at the membrane surface (psi).

To relate the osmotic pressure to the brine concentration, Merten, et al. (40), has found that the expression

$$\pi_S^n = 12{,}100 \; \hat{x}_s^n \text{ (psi)} \tag{12}$$

fits the experimental data of Tribus, et al. (41), where $\hat{x}_s^n$ is the average mass fraction of salt concentration at the membrane surface of the nth stage.

Now let us apply the boundary-layer flow analysis to the nth stage. The pressure is uniform in the high pressure chamber if the pressure drop due to bulk flow is negligible. A salt material balance inside the concentration boundary layer for a plane parallel to the membrane is described as follows.

$$-D_a \frac{d\hat{x}^n}{dy} = F^n \frac{\hat{x}^n}{1 - \hat{x}^n} \tag{13}$$

where $D_a \dfrac{d\hat{x}^n}{dy}$ is the rate of migration of salt component in the direction from the membrane surface to the main bulk solution by diffusion, and $F^n \dfrac{\hat{x}^n}{1 - \hat{x}^n}$ is the volumetric flow rate of salt in the direction from the main bulk solution to the membrane surface by bulk motion or convection.

Therefore

$$-\frac{d\hat{x}^n}{dy} = \frac{F^n}{D_a} \frac{\hat{x}^n}{1 - \hat{x}^n} \,. \tag{14}$$

Since

$$\hat{x}^n << 1, \quad \frac{\hat{x}^n}{1 - \bar{x}^n} \cong \hat{x}^n$$

equation (14) can be simplified to

$$-\frac{d\hat{x}^n}{\hat{x}^n} = \frac{F^n}{D_a} dy \,. \tag{15}$$

If we assume D_a to be independent of $\hat{x}^n$, integrating the right-hand side of equation (15) from 0 to $\delta_c^n \big|$ and the left-hand side from $\hat{x}_S^n$ to $\hat{x}^n$ yields

$$\int_{\hat{x}^n}^{\hat{x}_S^n} \frac{d\hat{x}^n}{\bar{x}^n} = \frac{F^n}{D_a} \int_0^{\delta_c^n} dy$$

or

$$\ln \frac{\hat{x}_S^n}{\hat{x}^n} = \frac{F^n}{D_a} \delta_c^n . \tag{16}$$

Substituting the concentration boundary-layer thickness, equation (7a), into equation (16), we have

$$\ln = \frac{\hat{x}_S^n}{\hat{x}^n} = \frac{F^n}{D_a} \frac{25.2\ d}{(Sc)^{1/3}\ (Re^n)^{7/8}} . \tag{17}$$

If we use the approximation

$$\ln \frac{\hat{x}_S^n}{\hat{x}^n} \cong \left(\frac{\hat{x}_S^n}{\hat{x}^n} - 1\right) \tag{18}$$

in equation (17) and solve for F^n, we obtain

$$F^n = \left(\frac{\hat{x}_S^n}{\hat{x}^n} - 1\right) \frac{(Sc)^{1/3}\ (Re^n)^{7/8}\ D_a}{25.2\ D} . \tag{19}$$

Substituting equations (19) and (12) into equation (11) and solving for $\hat{x}_S^n$, we obtain

$$\hat{x}_S^n = \frac{\hat{x}^n \left(1 + K\Delta P^n \dfrac{25.2\ d}{(Sc)^{1/3}\ (Re^n)^{7/8}\ D_a}\right)}{1 + 12{,}100\ \hat{x}^n\ K \dfrac{25.2\ d}{(Sc)^{1/3}\ (Re^n)^{7/8}\ D_a}} . \tag{20}$$

Substituting equation (20) into equation (19), we obtain the volumetric flow rate of fresh water per unit area of membrane from the nth stage as

$$F^n = \frac{K(\Delta P^n - 12,100\ \hat{x}^n)}{1 + 12,100\ \hat{x}^n\ K \dfrac{25.2\ d}{(Sc)^{1/3}\ (Re^n)^{7/8}\ D_a}}$$

$$= \frac{K(\Delta P^n - 12,100\ \hat{x}^n)}{1 + C \dfrac{\hat{x}^n}{(Re^n)^{7/8}}} \left(\frac{ft^3}{ft^2 - hr}\right) \qquad (21)$$

where

$$C = 12,100\ K \frac{25.2\ d}{(Sc)^{1/3}\ D_a}$$

$$= 3.05 \times 10^5 \frac{K\ d}{(Sc)^{1/3}\ D_a} . \qquad (22)$$

The overall material balance around the nth stage is

$$q^n = q^{n-1} - W^n . \qquad (23)$$

Thus the fresh water produced from the nth stage is

$$W^n = F^n \rho S^n \qquad (23a)$$

where S^n is the membrane area of the nth stage (ft^2) and ρ is the density of the fresh water $(\frac{lb_m}{ft^3})$.

The salt balance around the nth stage is

$$q^0 x^0 = q^n \hat{x}^n$$

or

$$\hat{x}^n = \frac{q^0 x^0}{q^n}$$

$$= \frac{q^0 x^0}{q^{n-1} - F^n \rho S^n}$$

$$= \frac{q^0 x^0}{\frac{x^0 q^0}{\hat{x}^{n-1}} - F^n \rho S^n}$$

$$= \frac{x^0 x^{n-1}}{x^0 - \hat{x}^{n-1} F^n \rho (\frac{S^n}{q^0})} . \qquad (24)$$

4. Relation Between the Reynolds Number Re^n and the Recycle Ratio R^n

The cross-sectional area through which the brine solution passes at the nth stage, A^n (note that this is different from the membrane area S^n), depends on the design of the separator unit at each stage. Often it is economical to use unifying equipment at each stage; thus we use at every stage a set of m-tubes arranged parallel to each other as a separator unit. Then the cross-sectional area remains the same at each stage and can be given in terms of the diameter of the tubes as

$$A^n = A = \frac{m\pi(d)^2}{4} . \qquad (25)$$

Similarly, $S^n - S$ for all stages.

The fluid velocity inside the tubes of the nth stage is

$$\hat{u}^n = \frac{q^{n-1}(1 + R^n)}{A \rho}$$

$$= \frac{4q^{n-1}(1 + R^n)}{m\pi(d)^2 \rho} . \qquad (26)$$

The relation between the Reynolds number Re^n and the recycle ratio R^n at the nth stage is

$$Re^n = \frac{d\, u^n \rho}{\mu} = \frac{d \rho}{\mu} \frac{4q^{n-1} (1 + R^n)}{\rho m \pi (d)^2}$$

$$= \frac{4q^{n-1} (1 + R^n)}{\mu m \pi d} . \qquad (27)$$

Substituting $q^{n-1} = \dfrac{q^0 x^0}{x^{n-1}}$ into equation (27), we obtain

$$Re^n = \frac{4q^0 x^0}{\mu m\ x^{n-1}\ d\pi} (1 + R^n) . \qquad (28)$$

CHAPTER IV. COST ANALYSIS

1. Operating Cost

Energy requirements per lb_m of fresh water product can be determined as follows.

Let us consider any two successive stages as shown in Fig. 5. E_1^n represents the pumping work of the high pressure pump at the nth stage and E_2^n represents the pumping work of the circulation pump at the nth stage.

Let η_m, η_p, and η_r be the mechanical, pump, and turbine efficiencies, and η_f the loss factor.

A. <u>Energy Requirement for the High Pressure Pump at the nth Stage</u>. The pumping work E_1^n is primarily used to increase the pressure from P^{n-1} to P^n. Since the velocity difference between the two successive stages is small, the kinetic energy losses and friction energy losses can be included in the pump efficiency. Thus the power requirement for high pressure

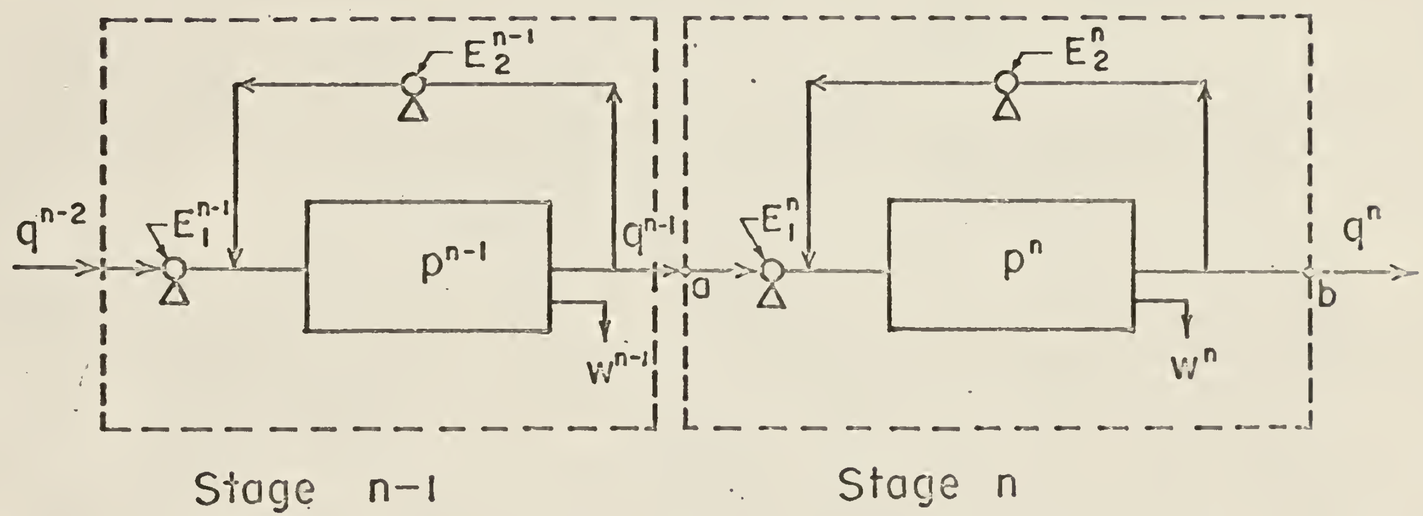

Fig. 5. Schematic diagram of two successive stages of a sequential reverse osmosis desalination process.

pumping at the nth stage, E_1^n, is

$$E_1^n = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{P^n - P^{n-1}}{\rho} q^{n-1} \left(\frac{\text{psi - ft}^3}{\text{hr}}\right) . \tag{29}$$

For one lb_m of total fresh water produced, we have

$$\frac{E_1^n}{W_f} = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{P^n - P^{n-1}}{\rho} \frac{q^{n-1}}{W_f} \left(\frac{\text{psi - ft}^3}{\text{lb}_m}\right) . \tag{30}$$

Substituting equations (9) and (10) into equation (30) yields

$$\frac{E_1^n}{W_f} = \frac{1 + \eta_f}{\eta_m \eta_p} \frac{P^n - P^{n-1}}{\rho} \frac{\frac{q^0 x^0}{x^{n-1}}}{q^0 (1 - \frac{x^0}{x^N})}$$

$$= \frac{1 + \eta_f}{\eta_m \eta_p} \frac{P^n - P^{n-1}}{\rho} \frac{x^0}{x^{n-1}(1 - \frac{x^0}{x^N})}$$

$$= \frac{1 + \eta_f}{\eta_m \eta_p} \frac{\Delta P - \Delta P^{n-1}}{\rho} \frac{x^0}{x^{n-1}(1 - \frac{x^0}{x^N})} . \tag{31}$$

B. <u>Energy Requirement for the Recycle Pump at the nth Stage</u>. The energy required, E_2^n, includes the energy of circulating the $q^{n-1}R^n$ lb_m/hr of fluid and that of the q^{n-1} flow work. The friction loss comes largely from the fluid flowing in the membrane separator unit. This lost work is (42)

$$E_2^n = 4f \frac{(\hat{u}^n)^2}{2g_c} \left(\frac{L}{d}\right) q^{n-1}(1 + R^n) \frac{1 + \eta_f}{\eta_m \eta_p} \tag{32}$$

where f is the friction factor, L is the length of the membrane separator unit, and d is the tube diameter of the membrane separator unit. $q^{n-1}(1 + R^n)$ is the amount of fluid flowing through the membrane separator unit, which is equal to

$$q^{n-1}(1 + R^n) = m \frac{\pi d^2}{4} \hat{u}^n \tag{33}$$

where m is the total number of tubes inside each membrane separator unit as mentioned previously.

As discussed before, the fluid flow within the membrane separator chamber would be in turbulent flow. Under this condition, the friction factor can be approximated by (43)

$$f = \frac{0.046}{(Re^n)^{0.2}} \quad . \tag{34}$$

Thus for one lb_m of fresh water produced, the energy required for the recycle pump is

$$\frac{E_2^n}{W_f} = \frac{4(0.046)}{(Re^n)^{0.2}} \cdot \frac{(u^n)^2}{2g_c} \left(\frac{L}{d}\right) \cdot \frac{m\pi (d)^2\, \bar{u}^n \rho}{4W_f} \; \frac{1 + \eta_f}{\eta_m \eta_p}$$

$$= \frac{0.023}{(Re^n)^{0.2}} \left(\frac{d\bar{u}^n \rho}{\mu}\right)^3 \left(\frac{\mu}{d\rho}\right)^3 \frac{Lm\pi d\,\rho}{g_c W_f} \; \frac{1 + \eta_f}{\eta_m \eta_p} \quad . \tag{35}$$

Note that $Lm\pi d$ is equal to the membrane surface area S, and $\frac{du^n \rho}{\mu} = Re^n$. By using equations (9) and (10), equation (35) becomes

$$\frac{E_2^n}{W_f} = 0.023\, (Re^n)^{2.8} \left(\frac{\mu}{d\rho}\right)^3 \frac{S\rho}{q^0\left(1 - \frac{x^0}{x^N}\right)} \; \frac{1 + \eta_f}{g_c \eta_m \eta_p} \quad . \tag{36}$$

C. Energy Recovery at Reject-brine Turbine. The equation for the energy recovery from depressurizing the high pressure brine solution will be of the same form as equation (30) which gives the energy requirement to pressurize the brine solution.

Thus we have

$$\frac{E_3}{W_f} = \eta_p \eta_m \, (1 - \eta_f) \, \frac{P^N - P^O}{\rho} \cdot \frac{q^N}{W_f}$$

$$= \eta_p \eta_m \, (1 - \eta_f) \, \frac{\Delta P^N}{\rho} \, \frac{\dfrac{x^O}{x^N}}{(1 - \dfrac{x^O}{x^N})} \qquad (37)$$

$$= \eta_p \eta_m \, (1 - \eta_f) \, \frac{\Delta P^N}{\rho} \, \frac{x^O}{x^N - x^O} \qquad (37)$$

where P^O is the discharge pressure (usually it is one atmosphere).

If the energy required is supplied from electricity the electrical power cost, C_e, is assumed to be \$0.005 per kw-hr in all cases.

2. Capital Cost

A. Pump and Turbine Installation Cost, C_p. For simplicity the costs of pump, turbine, and motor are assumed to be directly proportional to horsepower rating in the horsepower range of interest. An f.o.b. cost of \$100 per kw has been assumed by Merten, et al.(34).

B. Membrane Separator Unit Cost. Because of a lack of information about the cost of this type of equipment, the cost equation which Merten, et al. (34) derived is used. It is

$$\frac{W_S^n}{W^n} = \left(\frac{\rho_m d}{\sigma_m}\right) \left(\frac{\Delta p^n}{\rho_F{}^n}\right) \left(1.62 + \frac{0.54}{L/D} + \frac{0.189}{L/D} \sqrt{\frac{\sigma_m}{\Delta p^n}}\right) \qquad (38)$$

where

W_S^n = the mass of the shell-and-tube membrane separator unit of nth stage (lb_m)

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

σ_m = the allowable stress of the material of construction (psi)

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

W^n = the fresh water produced from the nth stage.

Changing equation (38) into the cost per lb_m of the fresh water produced, we have

$$\frac{W_S^n}{W_f} = \frac{W^n}{W_f} \cdot \frac{W_S^n}{W^n} = \left(\frac{\rho_m d}{\sigma_m}\right)\left(\frac{\Delta p^n}{F^n \rho}\right)\left(1.62 + \frac{0.54}{L/D} + \frac{0.189}{L/D}\sqrt{\frac{\sigma_m}{p^n}}\right)\frac{W^n}{W_f} \quad . \tag{39}$$

By using equations (9), (10), and (23a), equation (39) becomes

$$\frac{W_S^n}{W_f} = \left(\frac{\rho_m d}{\sigma_m}\right)\left(\frac{\Delta p^n}{F^n \rho}\right)\left(1.62 + \frac{0.54}{L/D} + \frac{0.189}{L/D}\sqrt{\frac{\sigma_m}{\Delta p^n}}\right)\frac{F^n S \rho}{q^0\left(1 - \frac{x^0}{x^N}\right)}$$

$$= \frac{\rho_m d}{\sigma_m}\;\frac{S\Delta p^n}{q^0\left(1 - \frac{x^0}{x^N}\right)}\left(1.62 + \frac{0.54}{L/D} + \frac{0.189}{L/D}\sqrt{\frac{\sigma_m}{\Delta p^n}}\right) \quad . \tag{40}$$

We assume that the cost of the membrane separator unit, which includes fabrication and installation costs, is proportional to the weight of the material used. And the unit cost of the material of construction is C_s \$/lb.

The annual capitalization charge for these equipment items is calculated at 0.074 of the initial cost per year, as recommended in the Office of Saline Water Report (44). An assumption of a load factor of 330-on-stream days per year gives a capitalization charge, Ψ, of 9.4×10^{-6} of initial cost per hour on stream.

The total cost contributions of the system are in the form

$$C_t = (\Psi C_p + C_e)\left(\sum_{n=1}^{N} \frac{E_1^n}{W_f} + \sum_{n=1}^{N} \frac{E_2^n}{W_f}\right) + (\Psi C_p - C_e)\frac{E_3}{W_f} + \Psi C_S \sum_{n=1}^{N} \frac{W_S^n}{W_f} \;. \tag{41}$$

Substituting equations (31), (36), (37), and (40) into equation (41) and combining all constants, we have

$$C_t = B_1 \frac{x^0}{1 - \frac{x^0}{x^N}} \sum_{1}^{N} \frac{\Delta P^n - \Delta P^{n-1}}{x^{n-1}} + \left(\frac{S}{q^0}\right)\left(\frac{x^N}{x^N - x^0}\right)\left\{B_2 \sum_{1}^{N} (Re^n)^{2.8} + B_3 \sum_{1}^{N} \Delta P^n + B_4 \sum_{1}^{N} (\Delta P^4)^{1/2}\right\} + B_5 \frac{x^0}{x^N - x^0} \Delta P^n \tag{42}$$

where

$$B_1 = (\Psi C_p + C_e)\frac{1 + \eta_f}{\rho \eta_m \eta_p} \tag{43}$$

$$B_2 = 0.023\,(\Psi C_p + C_e)\frac{1 + \eta_f}{g_c \eta_m \eta_p}\,\rho\left(\frac{\mu}{d\rho}\right)^3 \tag{44}$$

$$B_3 = \frac{\Psi C_s \rho_m d}{\sigma_m}\left(1.62 + \frac{0.54}{L/D}\right) \tag{45}$$

$$B_4 = \frac{0.189\,\Psi C_s \rho_m d}{\sqrt{\sigma_m}\; L/D} \tag{46}$$

$$B_5 = (\Psi C_p - C_e)\,\eta_p \eta_m (1 - \eta_f) / \rho \;. \tag{47}$$

CHAPTER V. CONCEPTUAL DESIGN

1. Assumptions

(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 tubes used m, are chosen arbitrarily.

(b) Each stage is geometrically similar. The membrane of each stage, S, is identical.

(c) Salt concentration of fresh water produced is assumed to be equal to zero, i.e., salt components cannot pass through the membrane.

(d) Feed saline water solution contains 3.5 weight per cent of salt components (average).

(e) The system is isothermal, and there is no precipitation of salts on the membrane surface.

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

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

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

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

2. System Variables and Number of System Variables (for the Total N Stages)

(a) Mass flow rate of brine solution.

$q^0, q^1, q^2, \ldots, q^N$; $N + 1$

(b) Salt concentration.

$x^1, x^2, \ldots, x^N$; N

(c) Operating pressure at each stage.

$p^1, p^2, \ldots, p^N$; N

(d) Fresh water produced from each stage.

$W^1, W^2, \ldots, W^N$; N

(e) Recycle rate of each stage.

$R^1, R^2, \ldots, R^N$; N

(f) Membrane area of one unit.

S 1

Total number of system variables = 5N + 2.

3. Relations and Number of Relations Among Various Variables

(a) Total material balance at each stage.

$$\left.\begin{array}{l} q^0 = W^1 + q^1 \\ q^1 = W^2 + q^2 \\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ q^{N-1} = W^N + q^N \end{array}\right\} N$$

(b) Salt material balance at each stage.

$$q^0 x^0 = q^1 x^1 = q^2 x^2 = \ldots = q^N x^N \; ; \qquad N$$

(c) Mass transfer at each stage.

$$\left.\begin{aligned}
W^1 = s\rho F^1 &= \frac{S\rho K(\Delta p^1 - 12{,}100\ \bar{x}^1)}{1 + C\dfrac{\bar{x}^1}{(Re^1)^{7/8}}} \\
W^2 = S\rho F^2 &= \frac{S\rho K(\Delta p^2 - 12{,}100\ \bar{x}^2)}{1 + C\dfrac{\bar{x}^2}{(Re^2)^{7/8}}} \\
&\cdots\cdots\cdots\cdots\cdots\cdots \\
&\cdots\cdots\cdots\cdots\cdots\cdots \\
&\cdots\cdots\cdots\cdots\cdots\cdots \\
W^N = S\rho F^N &= \frac{S\rho K(\Delta p^N - 12{,}100\ \bar{x}^N)}{1 + C\dfrac{\bar{x}^N}{(Re^N)^{7/8}}} \ .
\end{aligned}\right\}\ N$$

The total number of relations is thus 3N. The number of independent variables is calculated as follows:

Total variables - total relations

$$= 5N + 2 - 3N = 2N + 2 \ .$$

Note that from the design equations and cost function we can see that S and q^0 always appear together in the term (S/q^0). If we use (S/q^0) as a single variable in place of S and q^0, we can reduce by one variable the total number of independent variables. Thus the total of independent variables becomes 2N + 1. The mechanical, pump, and turbine efficiencies, η_m, η_p, η_r, are all treated as parameters.

4. Illustrative Examples

The following data are used:

$D_a = 1.5 \times 10^{-5}$ cm^2/sec, the diffusion constant for Nacl in water at room temperature (46)

$K = 0.86 \times 10^{-4} \dfrac{ft^3}{ft^2 - hr - psi}$ (34)

$\nu = 8 \times 10^{-3} \dfrac{cm^2}{sec}$ for the brines at $30^\circ C$ (47)

$\rho = 62.4\ lb_m/ft^3$

$d = \dfrac{1}{24}$ ft

$L/D = 8$ (34)

$\rho_m = 2.7 \times 62.4\ lb_m\ ft^3$ density of aluminum (43)

$\sigma_m = 15{,}000$ psi, allowable stress of aluminum (43)

$\psi = 9.4 \times 10^{-6}\ hr^{-1}$

$C_p = 100$ \$ per kw (34)

$C_e = 0.005$ \$ per kw-hr (34)

$C_s = 4.4$ \$ per lb_m of aluminum (34)

$\eta_m = 0.9$

$\eta_r = \eta_p = 0.8$

$\eta_f = 0.1$.

Calculation of the constants is carried out as follows:

$$Sc^{1/3} = \left(\frac{\nu}{D_a}\right)^{1/3} = \left(\frac{8 \times 10^{-3}}{1.5 \times 10^{-5}}\right)^{1/3} = 8.1$$

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

$$= \frac{3.05 \times 10^5 \ psi \times 0.86 \times 10^{-4} \ \frac{ft^3}{ft^2\text{-}hr\text{-}psi} \times \frac{1}{24} \ ft}{8.1 \times 1.5 \times 10^{-5} \ \frac{cm^2}{sec} \times \frac{3600 \ sec}{hr} \times 0.001076 \ \frac{ft^2}{cm^2}}$$

$$= 2.32 \times 10^3$$

$$B_1 = (\Psi C_p + C_e) \ \frac{1 + \eta_f}{\rho \ \eta_m \eta_p}$$

$$= (9.4 \times 10^{-6} \ \frac{1}{hr} \times 100 \ \frac{\$}{kw}$$

$$+ 0.005 \ \frac{\$}{kw\text{-}hr}) \ \frac{1 + 0.1}{62.4 \ \frac{lb_m}{ft^3} \times 0.9 \times 0.8}$$

$$\times 3.766 \times 10^{-7} \ \frac{kw\text{-}hr}{ft\text{-}lb} \times (\frac{12 \ in}{ft})^2$$

$$= 0.7887 \times 10^{-8} \ (\frac{\$}{psi\text{-}lb_m})$$

$$B_2 = 0.023 \ (9.4 \times 10^{-6} \times 100 + 0.005) \ \frac{\$}{kw\text{-}hr}$$

$$\times \frac{1 + 0.1}{0.9 \times 0.8 \times 32.2} \ (\frac{lb_f\text{-}sec^2}{lb_m\text{-} \ ft})$$

$$\times 62.4 \ \frac{lb_m}{ft^3} \times (\frac{8 \times 10^{-3} \ \frac{cm^2}{sec}}{1/24 \ ft} \ \times 0.001076 \ \frac{ft^2}{cm^2})^3$$

$$\times 3.766 \times 10^{-7} \ \frac{kw\text{-}hr}{lb_f\text{-}ft} \times 3600 \ \frac{sec}{hr}$$

$$= 0.4835 \times 10^{-17} \left(\frac{\$}{ft^2\text{-}hr}\right)$$

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

$$= \frac{9.4 \times 10^{-6}\ hr^{-1} \times 4.4 \dfrac{\$}{lb_m} \times 2.7 \times 62.4 \dfrac{lb_m}{ft^3} \times \dfrac{1}{24}\ ft}{15{,}000\ psi} \left(1.62 + \frac{0.54}{8}\right)$$

$$= 0.3266 \times 10^{-7} \left(\frac{\$}{psi\text{-}ft^2\text{-}hr}\right)$$

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

$$= \frac{0.189 \times 9.4 \times 10^{-6} \times 4.4 \dfrac{\$}{hr\text{-}lb_m} \times 2.7 \times 62.4 \dfrac{lb_m}{ft^3} \times \dfrac{1}{24}\ ft}{\sqrt{15{,}000\ psi} \times 8}$$

$$= 0.133 \times 10^{-6} \left(\frac{\$}{\sqrt{psi\text{-}ft^2\text{-}hr}}\right)$$

$$B_5 = (\psi C_p - C_e)\, \eta_p\, \eta_m\, (1 - \eta_f)/\rho$$

$$= (9.4 \times 10^{-6} \times 100 - 0.005) \frac{\$}{kw\text{-}hr} \times 0.9 \times 0.8 \times (1 - 0.1)$$

$$\times \frac{1\ ft^3}{62.4\ lb_m} \times 3.766 \times 10^{-7} \frac{kw\text{-}hr}{lb_f\text{-}ft} \times \left(\frac{12\ in}{ft}\right)^2$$

$$= -0.2286 \times 10^{-8} \left(\frac{\$}{lb_m - psi}\right).$$

In this illustrative example, the average salt concentration within the membrane separator chamber of the nth stage $\hat{x}^n$ is assumed to be equal to the salt concentration in the outlet brine solution of the nth stages x^n.

From equation (25), we see that this assumption is valid for high recycle ratio; thus equation (21) becomes

$$F^n = \frac{K(\Delta p^n - 12{,}100\ x^n)}{1 + C \dfrac{x^n}{(Re^n)^{7/8}}} \quad . \tag{50}$$

Substituting equation (50) into equation (24) and simplifying, we obtain

$$x^n \left\{ \frac{1}{x^{n-1}} \quad \frac{s}{q^0} \quad \frac{}{x^0} \quad \frac{K(\Delta p^n - 12{,}100\ x^n)}{1 + C \dfrac{x^n}{(Re^n)^{7/8}}} \right\} = 1 \ . \tag{51}$$

A. <u>Calculation of the Cost for a 3-stage System for Various Recycle Ratios but with the Same Operating Pressure at Each Stage</u>.

The total number of independent variables is

$2N + 1 = 7$.

By choosing the Reynolds number for each stage as

$Re^1 = .97 \times 10^4$

$Re^2 = 1.94 \times 10^4$

$Re^3 = 2.9 \times 10^4$,

the operating pressure drop as

$P^1 = P^2 = P^3 = 1014.7$ psi

or $\Delta P^1 = \Delta P^2 = \Delta P^3 = 1{,}000$ psi,

and the discharged concentration as

$x^3 = 0.071$,

then the whole system will be fixed. Note that using the Reynolds number at each stage as an independent variable renders the calculations easier than using the recycle ratio as an independent variable.

The values of the Reynolds number used are based on the assumption that the fluid velocities in the separator chamber are

$$U^1 = 2 \text{ ft/sec}$$
$$U^2 = 4 \text{ ft/sec}$$
$$U^3 = 6 \text{ ft/sec.}$$

The corresponding values of $(Re^n)^{7/8}$, n = 1, 2, 3, are

$$(Re^1)^{7/8} = (0.97 \times 10^4)^{7/8} = 3.08 \times 10^3$$
$$(Re^2)^{7/8} = (1.94 \times 10^4)^{7/8} = 5.61 \times 10^3$$
$$(Re^3)^{7/8} = (2.9 \times 10^4)^{7/8} = 8.04 \times 10^3 \ .$$

Substituting the known values into equation (51), we have

$$x^1 \left\{ \frac{1}{0.035} - \left(\frac{S}{q^0}\right) \frac{ft^2}{lb_m/hr} \cdot \frac{62.4 \frac{lb_m}{ft^3}}{0.035} \cdot \frac{0.86 \times 10^{-6} \frac{ft^3}{ft^2\text{-hr-psi}} (1000 - 12,100\ x^1)\text{psi}}{1 + 2.32 \times 10^3 \frac{x^1}{3.08 \times 10^3}} \right\} = 1$$

and

$$x^2 \left\{ \frac{1}{x^1} - \left(\frac{S}{q^0}\right) \frac{ft^2}{lb_m/hr} \frac{62.4 \frac{lb_m}{ft^3}}{0.035} \cdot \frac{0.86 \times 10^{-4} \frac{ft^3}{ft^2\text{-hr-psi}} (1000 - 12,100\ x^2)\text{psi}}{1 + 2.32 \times 10^3 \frac{x^2}{5.61 \times 10^3}} \right\} = 1$$

and

$$0.071 \left\{ \frac{1}{x^2} - \left(\frac{S}{q^0}\right) \frac{ft^2}{lb_m/hr} \; \frac{62.4 \dfrac{lb_m}{ft^3}}{0.035} \; \frac{0.86 \times 10^{-4} \dfrac{ft^3}{ft^2\text{-hr-psi}} (1000 - 12{,}000 \times 0.071)}{1 + 2.32 \times 10^{-3} \dfrac{0.071}{9.04 \times 10^3}} \right\} = 1 \; .$$

By trial and error we can solve these three equations with three unknowns. The results are

$$\frac{S}{q^0} = 0.11 \; \frac{ft^2}{lb_m/hr}$$

$$x^1 = 0.047$$

$$x^2 = 0.06 \; .$$

Then we can calculate the cost for this system. First we calculate

$$\sum_{n=1}^{3} (Re^n)^{2.8} = (0.97 \times 10^4)^{2.8} + (1.94 \times 10^6)^{2.8} + (2.9 \times 10^4)^{2.8} = 4.385 \times 10^{12}$$

$$\sum_{n=1}^{3} (\Delta P^n) = 3{,}000 \text{ psi}$$

$$\sum_{n=1}^{3} (\Delta P^n)^{1/2} = 3 \times (1000)^{1/2} = 94.92 \sqrt{psi} \; .$$

Substituting these values into equation (42), we have

$$C_t = B_1 \frac{x^0}{1 - \dfrac{x^0}{x^N}} \sum_{1}^{N} \frac{\Delta P^n - \Delta P^{n-1}}{x^{n-1}} + \left(\frac{S}{q^0}\right) \frac{x^N}{x^N - x^0} \left\{ B_2 \sum_{1}^{N} (Re^n)^{2.8} \right.$$

$$+ B_3 \sum_1^N \Delta P^n + B_4 \sum_1^N (\Delta P^n)^{1/2}\} + B_5 \frac{x^0}{x^N - x^0} \Delta P^N$$

$$= 0.7887 \times 10^{-8} \frac{\$}{psi - lb_m} \frac{0.035}{1 - \frac{0.035}{0.071}} (\frac{1000 \text{ psi}}{0.035} + 0 + 0)$$

$$+ 0.11 \frac{ft^2}{lb_m/hr} (\frac{0.071}{0.071 - 0.035})(0.4835 \times 10^{-17} \frac{\$}{ft^2\text{-}hr}$$

$$\times 4.385 \times 10^{12} + 0.3266 \times 10^{-7} \frac{\$}{psi\text{-}ft^2\text{-}hr} \times 3000 \text{ psi}$$

$$+ 0.133 \times 10^{-6} \frac{\$}{\sqrt{psi\text{-}ft^2\text{-}hr}} \times 94.92 \sqrt{psi}$$

$$- 0.2286 \times 10^{-8} \frac{\$}{lb_m\text{-}psi} \times 1000 \text{ psi} \times \frac{0.035}{0.071 \times 0.035}$$

$$= 4.2255 \times 10^{-5} \frac{\$}{lb_m} = 0.3545 (\frac{\$}{1000 \text{ gal}}) .$$

B. <u>Calculation of the Cost for a System of Three Stages with a Stepwise Increase in the Recycle Ratio and Operating Pressure from Stage to Stage</u>.

As in (a), the system has seven independent variables. Here we use the same values of the Reynolds number as in (a). However, the operating pressure is increased from stage to stage, as follows.

$\Delta P^1 = 1000$ psi

$\Delta P^2 = 1250$ psi

$\Delta P^3 = 1500$ psi.

The discharging concentration is

$x^3 = 0.07$.

Then the system is fixed. Substituting these values into equation (51), we have

$$x^1 \left\{ \frac{1}{0.035} - \left(\frac{S}{q^0}\right) \frac{62.4}{0.035} \quad \frac{0.86 \times 10^{-4}\,(1000 - 12{,}100\ x^1)}{1 + 2.32 \times 10^3 \dfrac{x^1}{3.08 \times 10^3}} \right\} = 1$$

$$x^2 \left\{ \frac{1}{x^1} - \left(\frac{S}{q^0}\right) \frac{62.4}{0.035} \quad \frac{0.86 \times 10^{-4}\,(1250 - 12{,}100\ x^2)}{1 + 2.32 \times 10^3 \dfrac{x^2}{5.61 \times 10^3}} \right\} = 1$$

$$0.07 \left\{ \frac{1}{x^2} - \left(\frac{S}{q^0}\right) \frac{62.4}{0.035} \quad \frac{0.86 \times 10^{-4}\,(1500 - 12{,}100 \times 0.07)}{1 + 2.32 \times 10^3 \dfrac{0.07}{8.04 \times 10^3}} \right\} = 1.$$

By trial and error, we can solve these three equations with three unknowns, x^1, x^2, and $\frac{S}{q^0}$. The results are

$$x^1 = 0.041$$

$$x^2 = 0.051$$

$$\frac{S}{q^0} = 0.05 \frac{ft^2}{lb_m/hr} .$$

Calculating the cost for this system, we obtain

$$\sum_{n=1}^{3} (\Delta P^n) = 3750 \text{ psi}$$

$$\sum_{n=1}^{3} (\Delta P^n)^{1/2} = (1000)^{1/2} + (1250)^{1/2} + (1500)^{1/2}$$

$$= 105.7 \sqrt{\text{psi}}$$

$$\sum_{n=1}^{3} \frac{\Delta P^n - \Delta P^{n-1}}{x^{n-1}} = \frac{1000}{0.035} + \frac{250}{0.041} + \frac{250}{1.051}$$

$$= 3.957 \times 10^4 \text{ psi}$$

$$\sum_{n=1}^{3} (Re^n)^{2.8} = 4.385 \times 10^{12} .$$

Substituting the values computed into the cost function, equation (42), we have

$$C_t = 0.7887 \frac{0.035}{1 - \frac{0.035}{0.07}} 3.957 \times 10^4$$

$$+ 0.05 \left(\frac{0.07}{0.07 - 0.035}\right) (0.4835 \times 10^{-17} \times 4.385 \times 10^{12}$$

$$+ 0.3266 \times 10^{-7} \times 3750 + 0.133 \times 10^{-6} \times 105.7)$$

$$- 0.2286 \times 10^{-8} \times 1500$$

$$= 3.4192 \times 10^{-5} \frac{\$}{lb_m} = 0.2848 \left(\frac{\$}{1000 \text{ gal}}\right) .$$

C. <u>Calculation of the Cost for a One-stage System</u>. We have the total number of independent variables of this system

$$= 2 + 1 = 3.$$

(i) We choose the Reynolds number as (34)

$$Re = 15{,}600$$

the operating pressure as

$$\Delta P = 1000 \text{ psi}$$

and the discharged concentration as (34)

$$x^3 = 0.051 .$$

Then the whole system will be fixed.

Employing equation (51), we obtain

$$0.051 \left\{ \frac{1}{0.035} - \left(\frac{S}{q^0}\right) \frac{62.4}{0.035} \right.$$

$$\left.\frac{0.36 \times 10^{-4} (1000 - 12{,}100 \times 0.051)}{1 + \dfrac{2.32 \times 10^{3}}{(15{,}600)^{7/8}} 0.051}\right\} = 1$$

or

$$0.051 \left\{ 28.57 - \left(\frac{S}{q^0}\right) \frac{58.7084}{1.0254} \right\} = 1$$

or

$$(28.57 - 19.607) \frac{1.0254}{58.7084} = \frac{S}{q^0} = 0.1565 \ .$$

The cost function is

$$C_t = 0.7887 \times 10^{-8} \times \frac{0.035}{1 - \dfrac{0.035}{0.051}} \left(\frac{1000}{0.035}\right)$$

$$+ 0.1565 \times \left(\frac{0.051}{0.051 - 0.035}\right) \Big(0.4835 \times 10^{-17} \times (15{,}600)^{2.8}$$

$$+ 0.3266 \times 10^{-7} \times 1000 + 0.133 \times (1000)^{1/2} \times 10^{-6}\Big)$$

$$- 0.2286 \times 10^{-8} \frac{0.035}{0.051 - 0.035} \times 1000$$

$$= 3.9953 \times 10^{-5} \frac{\$}{lb_m} = 0.33281 \left(\frac{\$}{1000 \text{ gal}}\right) .$$

(ii) If we use the same Reynolds number and operating pressure, but use the discharging concentration at

$$x^1 = 0.07$$

we have

$$0.07 \left\{ \frac{1}{0.035} - \frac{S}{q^0} \frac{62.4}{0.035} \frac{0.86 \times 10^{-4} (1000 - 12{,}100 \times 0.07)}{1 + 2.32 \times 10^3 \dfrac{0.07}{4.6563 \times 10^3}} \right\} = 1$$

or

$$(28.57 - 14.285) / \left\{ \frac{62.4}{0.035} \frac{0.86 \times 10^{-4} \times 153}{1 + 0.0349} \right\} = \frac{S}{q^0}$$

or

$$\frac{S}{q^0} = \frac{14.285}{22.668} = 0.6302 \ .$$

The value of the cost function is

$$C_t = 0.7887 \times 10^{-8} \times \frac{0.035}{1 - \dfrac{0.035}{0.07}} \left(\frac{1000}{0.035}\right)$$

$$+ 0.6302 \left(\frac{0.07}{0.07 - 0.035}\right) \Big\{ 0.4835 \times 10^{-17} \times (15{,}600)^{2.8}$$

$$+ 0.3266 \times 10^{-7} \times 1000 + 0.133 \times (1000)^{1/2} \times 10^{-6} \Big\}$$

$$- 0.2286 \times 10^{-8} \frac{0.035}{0.07 - 0.035} \times 1000$$

$$= 6.355 \times 10^{-5} \frac{\$}{lb_m} = 0.5294 \left(\frac{\$}{1000 \text{ gal}}\right) \ .$$

From the first and second examples, we see that by using a gradually increasing operating pressure we can get the better result (i.e., lower cost) than by using the same operating pressure throughout the system. From the third example we can recognize that our proposed sequential process is better than the others. Although the processes presented in those examples are yet to be optimized completely, we believe that we still can get the qualitative conclusion that the proposed process is better than other processes operated under these similar operating conditions.

Since we have already formulated a system model or a set of system equations in previous chapters, we should be able to use the model to find the optimum design and operating conditions of the system. And since the proposed system has a set of well defined system equations, and the transformation functions are continuously differentiable with respect to the state variables, from the previous two parts, we see that the system can be optimized by means of the multi-level approach and/or the discrete maximum principle. The main difficulty in a numerical solution is the convergence of the iteration scheme. The choice of the step size factor, k, is a difficulty. If it is too large, the iteration scheme will not converge. Yet, if it is too small, convergence is extremely slow. The step size factor, k, can only be adjusted on a trial-and-error basis to achieve convergence. This needs a lot of computer time. This work will be left for future work.

NOMENCLATURE FOR PART THREE

A, A^n = Cross-section area normal to the streamline of any membrane separator unit, (ft^2).

C = $3.05 \times 10^5 \dfrac{K \cdot d}{Sc^{1/3}\, D_a}$ constant.

C_e = Electrical power cost (\$/kw-hr).

C_p = Pump and turbine installed cost (\$/kw).

C_s = The unit cost of the material for constructing membrane separator unit (\$/lb_m).

C_t = The total cost per pound of fresh water produced (\$/lb_m).

d = The diameter of the tubes in the membrane separator unit.

D_a = Molecular diffusion coefficient of salt $\left(\dfrac{sq\ cm}{sec}\right)$.

E_1^n = Pump work of high pressure pump at nth stage.

E_2^n = Pump work of circulation pump at nth stage.

E_3^n = Energy recovery from the blowdown turbine at the end of the process.

f = Fanning friction factor.

F^n = The volumetric flow rate of fresh water product through the membrane of nth stage $\left(\dfrac{ft^3}{ft^2 - hr}\right)$.

F_s^n = The volumetric flow rate of salt component through the membrane of nth stage $\left(\dfrac{ft^3}{ft^2 - hr}\right)$.

K = Membrane constant $\left(\dfrac{ft^3}{ft^2 - hr - psi}\right)$.

m = The total number of tubes within each membrane separator unit.

N = Total number of stages in the sequence of the process.

P^n = Pressure within membrane separator chamber of nth stage (psi).

P^0 = Atmosphere pressure (14.7 psi).

ΔP^n = $P^n - P^0$ = Pressure difference across the membrane at nth stage (psi).

q^n = Mass flow rate of brine solution discharged from nth stage (lb_m/hr).

q^0 = Mass flow rate of feed saline water (lb_m/hr).

R = The radius of the tubes within the membrane separator unit = 1/2 d.

R^n = Recycle ratio of nth stage.

Re^n = Average Reynolds number at nth stage.

S, S^n = Membrane area of one membrane separator unit (ft^2).

Sc = Schmidt number.

U = The maximum velocity within the membrane separator unit.

$\hat{u}$ = Mean velocity within the membrane separator unit = $0.8\ \hat{U}$ (for turbulent flow).

$\hat{u}^n$ = Mean velocity within the membrane separator chamber of nth stage.

v_* = Friction velocity.

W^n = Mass flow rate of fresh water produced from nth stage (lb_m/hr).

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

W_s^n = The mass of the shell-and-tube membrane separator unit of nth stage (lb_m).

x^n = The stage variable; here we denote the mass fraction of the salt component in the outlet brine solution of nth stage.

$\hat{x}^n$ = Average mass fraction of salt concentration within membrane separator chamber of nth stage.

$\hat{x}_3^n$ = Average mass fraction of salt concentration at the membrane surface of nth stage.

y = Distance normal to membrane boundary.

Greek Letters

δ = Momentum transport boundary-layer thickness.

δ_c = Mass transport boundary-layer thickness.

ν = Kinematic viscosity = $\frac{\mu}{\rho}$ $\left(\frac{\text{sq cm}}{\text{sec}}\right)$.

μ = Viscosity of brine solution.

ρ = Density of brine solution, (lb_m/ft^3).

ρ_m = Density of material of constriction (lb_m/ft^3).

θ^n = Decision variable of nth stage.

π_s^n = The osmotic pressure of the brine solution at the membrane surface of nth stage (psi).

τ_0 = Shearing stress at the wall.

η_f = Loss factor.

η_m = Mechanical efficiency.

η_p = Pump efficiency.

η_r = Turbine efficiency.

ψ = Capitalization charge of initial cost per hour in stream (\$/hr).

σ_m = Allowable stress of the material of construction (psi).

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APPENDIX

PROOF FOR THE CONVERGENCE OF THE PRICE-ADJUSTMENT RULE

Consider the nth subproblem. For some prices p^n, let those components of R^n which are zero at the subproblem extremum be the first r^n, $0 \leq r^n \leq \gamma^n$. That is, to separate $R^n \geq 0$ into equality and inequality parts,

$$R_i^n(\theta^n, y^{n,N+1}, x^{n-1}) = 0, \quad i = 1, 2, \ldots, r^n \tag{A.1a}$$

$$R_i^n(\theta^n, y^{n,N+1}, x^{n-1}) > 0, \quad i = r^n, r^n + 1, \ldots, \gamma^n . \tag{A.1b}$$

Define the Lagrangian for the nth subproblem as

$$L^n = S^n \sum_{j=1}^{r^n} u_j^n R_j^n . \tag{A.1}$$

Substituting the expression for the subobjective function S^n, equation (1.7), Chapter III, Part One, into this equation, the Lagrangian becomes

$$L^n = f^n(\theta^n, y^n) + (p^n)^T\, T(\theta^n, x^{n-1}) - (p^{n-1})^T x^{n-1} + (u^n)^T R^n(\theta^n, y^n, x^{n-1}) . \tag{A.2}$$

The solutions $\tilde{\theta}^n$, $\tilde{x}^{n-1}$, $\tilde{u}^n$ to this subproblem satisfy the following:

$$\frac{\partial L^n}{\partial \theta_k^n} = \frac{\partial f^n}{\partial \theta_k^n} + (p^n)^T \frac{\partial T^n}{\partial \theta_k^n} + (u^n)^T \frac{\partial R^n}{\partial \theta_k^n} = 0 \tag{A.3}$$

$$k = 1, 2, \ldots, w^n$$

$$\frac{\partial L^n}{\partial x_k^{n-1}} = \frac{\partial f^n}{\partial x_k^{n-1}} + (p^n)^T \frac{\partial T^n}{\partial x_k^{n-1}} - (u^n)^T \frac{\partial R^n}{\partial x_k^{n-1}} \tag{A.4}$$

$$k = 1, 2, \ldots, s^{n-1}$$

$$R_i^n = 0, \quad i = 1, 2, \ldots, r^n . \tag{A.5}$$

If the following independent small perturbation of p^n is made at each subsystem,

$$p^n = p^n + \Delta p^n , \qquad n = 1, 2, \ldots, N \tag{A.6}$$

the disturbance will alter the solutions of equations (A.3) through (A.5) to

$$\begin{aligned} &\tilde{x}^{n-1} + \Delta x^{n-1} \\ &\tilde{\theta}^n + \Delta \theta^{n-1} \end{aligned} \tag{A.7}$$

and

$$\tilde{u}^n + \Delta u^n .$$

The variational equations can be obtained from equations (A.3) through (A.5) as

$$\left(\frac{\partial f^n}{\partial \theta_k^n}\right)_\Delta + (p_0^n + \Delta p^n)^T \left(\frac{\partial T^n}{\partial \theta_k^n}\right)_\Delta + (u^n + \Delta u^n)^T \left(\frac{\partial R^n}{\partial \theta_k^n}\right)_\Delta = 0 \tag{A.8}$$

[1]

$$k = 1, 2, \ldots, w^n$$

$$\left(\frac{\partial f^n}{\partial x_k^{n-1}}\right)_\Delta + (p_0^n + \Delta p^n)^T \left(\frac{\partial R^n}{\partial x_k^{n-1}}\right)_\Delta - (p_0^{n-1} + \Delta p^{n-1})$$

$$+ (\tilde{u}^n + \Delta u^n)_\Delta \left(\frac{\partial R^n}{\partial x_k^{n-1}}\right)_\Delta = 0 \tag{A.9}$$

$$k = 1, 2, \ldots, s^{n-1}$$

$$(R_i^n)_\Delta = 0 , \quad i = 1, 2, \ldots, r^n . \tag{A.10}$$

The quantities in equations (A.8) through (A.10) are then expanded in the Taylor series to the first-order terms. A representative term in this expansion has the form

$$\left(\frac{\partial f^n}{\partial \theta_k^n}\right)_\Delta = \frac{\partial f^n}{\partial \theta_k^n} + \sum_{j=1}^{w^n} \frac{\partial^2 f^n}{\partial \theta_j^n \partial \theta_k^n} \Delta \theta_j^n$$

---

[1] $(\;)_\Delta$ denotes the quantities inside the bracket and is evaluated at the perturbed states.

$$+ \sum_{j=1}^{s^{n-1}} \frac{\partial^2 f^n}{\partial x_j^{n-1} \partial \theta_k^n} \Delta x_j^{n-1} + O(\varepsilon^2) \qquad \text{(A.11)}$$

where $O(\varepsilon^2)$ denotes the term including second-order and those of higher order.

When all terms in equation (A.8) are expanded in this manner, we obtain the following:

$$\frac{\partial f^n}{\partial \theta_k^n} + \sum_{j=1}^{w^n} \frac{\partial^2 f^n}{\partial \theta_j^n \partial \theta_k^n} \Delta \theta_j^n + \sum_{j=1}^{s^{n-1}} \frac{\partial^2 f^n}{\partial x_j^{n-1} \theta_j^n} \Delta x_j^{n-1}$$

$$+ \sum_{i=1}^{s^n} (p^n + \Delta p^n) \left\{ \frac{\partial T_i^n}{\partial \theta_k^n} + \sum_{j=1}^{w^n} \frac{\partial^2 T_i^n}{\partial \theta_j^n \partial \theta_k^n} \Delta \theta_j^n \right.$$

$$\left. + \sum_{j=1}^{s^{n-1}} \frac{\partial^2 T_i^n}{\partial x_j^{n-1} \partial \theta_k^n} \Delta x_j^{n-1} \right\}$$

$$+ \sum_{i=1}^{r^n} (u^n + \Delta u^n) \left\{ \frac{\partial R_i^n}{\partial \theta_k^n} + \sum_{j=1}^{w^n} \frac{\partial^2 R_i^n}{\partial \theta_j^n \partial \theta_k^n} \Delta o_j^n \right.$$

$$\left. + \sum_{j=1}^{s^{n-1}} \frac{\partial^2 R_i^n}{\partial x_j^{n-1} \partial \theta_k^n} \Delta x_j^{n-1} \right\}$$

$$+ O(\varepsilon^2) = 0 \ . \qquad \text{(A.12)}$$

A similar expression is obtained by expanding equation (A.9). Expansion of equation (A.10) gives

$$R_i^n + \sum_{j=1}^{w^n} \frac{\partial R_i^n}{\partial \theta_j^n} \Delta \theta_j^n + \sum_{j=1}^{s^{n-1}} \frac{\partial R_i^n}{\partial x_j^{n-1}} \Delta x_j^{n-1} + O(\varepsilon^2) = 0 \ . \qquad \text{(A.13)}$$

Since each of the first r^n components of R_i^n is zero at the original price p_0^n , equation (A.13) reduces to

$$\sum_{j=1}^{w^n} \frac{\partial R_i^n}{\partial \theta_j^n} \Delta \theta_j^n + \sum_{j=1}^{s^{n-1}} \frac{\partial R_i^n}{\partial x_j^{n-1}} \Delta x_j^{n-1} + O(\varepsilon^2) = 0 \qquad (A.14)$$

Collecting the coefficients of $\Delta \theta_j^n$ and x_j^{n-1} and ignoring all terms involving the product of two or more increments, $O(\varepsilon^2)$, on the assumption that all of the functions $f^n(\theta^n, y^n)$, $T^n(\theta^n, x^{n-1})$, and $R^n(\theta^n, y^n, x^{n-1})$ depend smoothly on x^{n-1} and θ^n, equation (A.12) becomes

$$\frac{\partial f^n}{\partial \theta_k^n} + \sum_{i=1}^{s^n} p_i^n \frac{\partial T_i^n}{\partial \theta_k^n} + \sum_{i=1}^{r^n} u_i^n \frac{\partial R_i^n}{\partial \theta_k^n} + \sum_{j=1}^{w^n} \left\{ \frac{\partial^2 f^n}{\partial \theta_j^n \partial \theta_k^n} + \sum_{i=1}^{s^n} p_i^n \frac{\partial^2 T_i^n}{\partial \theta_j^n \partial \theta_k^n} + \sum_{i=1}^{r^n} u_i^n \frac{\partial^2 R_i^n}{\partial \theta_j^n \partial \theta_k^n} \right\} \Delta \theta_j^n$$

$$+ \sum_{j=1}^{s^{n-1}} \left\{ \frac{\partial^2 f^n}{\partial x_j^{n-1} \partial \theta_k^n} + \sum_{i=1}^{s^n} p_i^n \frac{\partial^2 T_i^n}{\partial x_j^{n-1} \partial \theta_k^n} + \sum_{i=1}^{r^n} u_i^n \frac{\partial^2 R_i^n}{\partial x_j^{n-1} \partial \theta_k^n} \right\} \Delta x_j^{n-1}$$

$$+ \sum_{i=1}^{s^n} \Delta p_i^n \frac{\partial T_i^n}{\partial \theta_k^n} + \sum_{i=1}^{r^n} \Delta u_i^n \frac{\partial R_i^n}{\partial \theta_k^n} = 0 \ . \qquad (A.15)$$

From the subobjective function S^n, equation (2.5), it can be seen that

$$\frac{\partial^2 S^n}{\partial \theta_j^n \partial \theta_k^n} = \frac{\partial^2 f^n}{\partial \theta_j^n \partial \theta_k^n} + \{p^n\}^T \frac{\partial^2 T^n}{\partial \theta_j^n \partial \theta_k^n} \qquad (A.16)$$

$$\frac{\partial^2 S^n}{\partial x_j^{n-1}\,\partial \theta_k^n} = \frac{\partial^2 f^n}{\partial x_j^{n-1}\,\partial \theta_k^n} + \{p^n\}^T \frac{\partial^2 T^n}{\partial x_j^{n-1}\,\partial \theta_k^n} \quad . \tag{A.17}$$

By using equations (A.3), (A.16), and (A.17), we can simplify equation (A.15) to obtain

$$\sum_{j=1}^{w^n} \left\{\frac{\partial^2 S^n}{\partial \theta_j^n\,\partial \theta_k^n} + \{u^n\}^T \frac{\partial^2 R^n}{\partial \theta_j^n\,\partial \theta_k^n}\right\} \Delta\theta_j^n$$

$$+ \sum_{j=1}^{s^{n-1}} \left\{\frac{\partial^2 S^n}{\partial x_j^{n-1}\,\partial \theta_k^n} + \{u^n\}^T \frac{\partial^2 R^n}{\partial x_j^{n-1}\,\partial \theta_k^n}\right\} \Delta x_j^{n-1}$$

$$+ \{\Delta p^n\}^T \frac{\partial T^n}{\partial \theta_k^n} + \{\Delta u^n\}^T \frac{\partial R^n}{\partial \theta_k^n} = 0 \quad . \tag{A.18}$$

An analogous development applied to equation (A.9) gives

$$\sum_{j=1}^{w^n} \left\{\frac{\partial^2 S^n}{\partial \theta_j^n\,\partial x_k^{n-1}} + \{u^n\}^T \frac{\partial^2 R^n}{\partial \theta_j^n\,\partial x_k^{n-1}}\right\} \Delta\theta_j^n$$

$$+ \sum_{j=1}^{s^{n-1}} \left\{\frac{\partial^2 S^n}{\partial x_j^{n-1}\,\partial x_k^{n-1}} + \{u^n\}^T \frac{\partial^2 R^n}{\partial x_j^{n-1}\,\partial x_k^{n-1}}\right\} \Delta x_j^{n-1}$$

$$+ \{\Delta p^n\}^T \frac{\partial T^n}{\partial x_k^{n-1}} + \{\Delta u^n\}^T \frac{\partial R^n}{\partial x_k^{n-1}} = 0 \quad . \tag{A.19}$$

Now we define the following vectors and matrices:

$$\{Q^n\} = \left\{\frac{\theta^n}{x^{n-1}}\right\} = \{q_i^n\} \tag{A.20}$$

$$i = 1,\ 2,\ \ldots,\ w^n,\ w^n + 1,\ \ldots,\ w^n + s^{n-1}$$

$$(J^n) = \left(\frac{\partial^2 S^n}{\partial q_j^n \, \partial q_k^n}\right) = \left(\frac{\partial^2 S^n}{\partial q_k^n \, \partial q_j^n}\right) \tag{A.21}$$

$$(K_i^n) = \left(\frac{\partial^2 R_i^n}{\partial q_j^n \, \partial q_k^n}\right) = \left(\frac{\partial^2 R_i^n}{\partial q_k^n \, \partial q_j^n}\right) \tag{A.22}$$

$$(B^n) = (J^n) + \sum_{i=1}^{r^n} \tilde{u}_i^n \, K_i^n \tag{A.23}$$

$$j = 1, 2, \ldots, w^n + s^{n-1}$$
$$k = 1, 2, \ldots, w^n + s^{n-1}$$
$$i = 1, 2, \ldots, r^n .$$

Note, since (J^n) and (K_i^n) are symmetric, the matrix (B^n) is symmetric too. Let

$$\Delta p_i^n \neq 0$$

$$\Delta p_j^n = 0, \quad \text{for} \quad j \neq i$$

and

$$\Delta p_j^{n-1} = 0, \quad \text{for} \quad \text{all } j.$$

Then dividing equations (A.18) and (A.19) by Δp_i^n, taking the limit as $\Delta p_i^n \longrightarrow 0$, and using the definitions, equations (A.20) through (A.23), we obtain

$$(B^n) \left\{\frac{\partial Q^n}{\partial p_i^n}\right\} = -\left\{\frac{\partial T_i^n}{\partial Q^n}\right\} - \left(\frac{\partial R^n}{\partial Q^n}\right)^T \left\{\frac{\partial u^n}{\partial p_i^n}\right\} \tag{A.24}$$

and

$$\left(\frac{\partial R^n}{\partial Q^n}\right) \left\{\frac{\partial Q^n}{\partial p_i^n}\right\} = 0 \tag{A.25}$$

$$n = 1, 2, \ldots, N$$
$$i = 1, 2, \ldots, s^n .$$

Similarly, letting

$$\Delta p_i^{n-1} \neq 0$$

$$\Delta p_j^{n-1} = 0, \quad \text{for} \quad j \neq i$$

and

$$\Delta p_j^{n} = 0, \quad \text{for} \quad \text{all } j$$

dividing equations (A.18) and (A.19) by Δp_i^{n-1} and passing Δp_i^{n-1} to the limit, we obtain

$$(B^n) \left\{ \frac{\partial Q^n}{\partial p_i^{n-1}} \right\} = \left\{ D^{w^n+i} \right\} - \left(\frac{\partial R^n}{\partial Q^n}\right)^T \left\{ \frac{\partial u^n}{\partial p_i^{n-1}} \right\} \qquad (A.26)$$

and

$$\left(\frac{\partial R^n}{\partial Q^n}\right) \left\{ \frac{\partial Q^n}{\partial p_i^{n-1}} \right\} = 0 \qquad (A.27)$$

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

$$i = 1, 2, \ldots, s^{n-1}$$

$$j = 1, 2, \ldots, r^n$$

where D^{w^n+i} is the $(w^n + s^{n-1})$ dimensional unit vector with a one in the (w^n+i)th position.

Premultiplying equations (A.24) and (A.26) by $(B^n)^{-1}$ with the assumption B^n is nonsingular, and substituting the expressions for $\partial Q^n/\partial p_i^n$ and $\partial R^n/\partial p_i^{n-1}$ thus obtained into equations (A.25) and (A.27), we have

$$\left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T \left\{ \frac{\partial u^n}{\partial p_i^n} \right\} = - \left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left\{ \frac{\partial T_i^n}{\partial Q^n} \right\} \quad (A.28)$$

$$i = 1, 2, \ldots, s^n$$

and

$$\left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T \left\{ \frac{\partial u^n}{\partial p_i^{n-1}} \right\} = \left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left\{ D^{w^n+i} \right\} \quad (A.29)$$

$i = 1, 2, \ldots, s^{n-1}$

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

For simplicity, we define the following expressions:

$$(C^n) = \left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T \quad (A.30)$$

$$\left\{C_i^n\right\} = \left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left\{\frac{\partial T_i^n}{\partial Q^n}\right\} \quad (A.31)$$

$$\left\{F_i^n\right\} = \left(\frac{\partial R^n}{\partial Q^n}\right) (B^n)^{-1} \left\{D^{w^n+i}\right\} \quad (A.32)$$

where C^n is an r^n by r^n matrix, G_i^n is an r^n-dimensional column vector, and so is F_i^n. Note that since B^n is symmetric, C^n is also symmetric. Thus the relations, equations (A.28) and (A.29), become

$$(C^n) \left\{ \frac{\partial u^n}{\partial p_i^n} \right\} = - \left\{ G_i^n \right\} \quad (A.33)$$

$i = 1, 2, \ldots, s^n$

and

$$(C^n) \left\{ \frac{\partial u^n}{\partial p_i^{n-1}} \right\} = - \left\{ F_i^n \right\} \quad (A.34)$$

$i = 1, 2, \ldots, s^{n-1}.$

Premultiplying by $(C^n)^{-1}$, equations (A.33) and (A.34) become

$$\left\{\frac{\partial u^n}{\partial p_i^n}\right\} = -\ (C^n)^{-1}\ \{G_i^n\} \tag{A.35}$$

and

$$\left\{\frac{\partial u^n}{\partial p_i^{n-1}}\right\} = (C^n)^{-1}\ \{G_i^n\} \tag{A.36}$$

Premultiplying by $(B^n)^{-1}$ and making use of equations (A.35) and (A.36), equations (A.24) and (A.26) become

$$\left\{\frac{\partial Q^n}{\partial p_i^n}\right\} = -\ (B^n)^{-1}\left\{\frac{\partial T_i^n}{\partial Q^n}\right\} + (B^n)^{-1}\ \left(\frac{\partial R^n}{\partial Q^n}\right)^T\ (C^n)^{-1}\ \{G_i^n\} \tag{A.37}$$

$$i = 1,\ 2,\ \ldots,\ s^n$$

$$\left\{\frac{\partial Q^n}{\partial p_i^{n-1}}\right\} = (B^n)^{-1}\ \{D^{w^n+i}\}\ -\ (B^n)^{-1}\ \left(\frac{\partial R^n}{\partial Q^n}\right)^T\ (C^n)^{-1}\ \{F_i^n\} \tag{A.38}$$

$$i = 1,\ 2,\ \ldots,\ s^{n-1}.$$

Now, in order to obtain the elements of $\frac{\partial E}{\partial P}$, we return to the definition of the vector of excess demand defined as (see equation (1.76, Chapter III, Part One),

$$E^n(P) = \tilde{x}^n - T^n(\tilde{\theta}^n,\ \tilde{x}^{n-1}).$$

Taking the first partial derivatives of $E^n(P)$ with respect to p^m, yields[1]

$$\frac{\partial E^n}{\partial p^m} = \frac{\partial \tilde{x}^n}{\partial p^m} - \frac{\partial T^n(\tilde{\theta}^n,\ \tilde{x}^{n-1})}{\partial p^m} \tag{A.39}$$

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

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

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[1]Recall that $P = (p^1\colon p^2\colon \ldots \colon p^N)$ is a matrix and p^n, $n = 1, 2, \ldots, N$, is a column vector.

From the necessary conditions for the subproblem to be extremized, equations (A.3), (A.4), and (A.5), it can be recognized that the nth subproblem solutions $\tilde{x}^{n-1}$, $\tilde{\theta}^n$, and $\tilde{u}^n$ are the functions of p^n and p^{n-1}. And since the solutions $\tilde{x}^n$ are determined by the (n+1)th subsystem, and they are only dependent on the values of p^n and p^{n+1}, and not dependent on the value of p^{n-1}. Thus the only nonvanishing terms of $\frac{\partial E^n}{\partial p^m}$ are those where $m = n-1$, n, and $n+1$. They are:

$$\frac{\partial E^n}{\partial p^{n-1}} = \frac{\partial \tilde{x}^n}{\partial p^{n-1}} - \frac{\partial T^n(\tilde{x}^{n-1}, \tilde{\theta}^n)}{\partial p^{n-1}} = - \frac{\partial T^n(\tilde{x}^{n-1}, \tilde{\theta}^n)}{\partial p^{n-1}} \tag{A.40}$$

$$n = 2, 3, \ldots, N$$

$$\frac{\partial E^n}{\partial p^n} = \frac{\partial \tilde{x}^n}{\partial p^n} - \frac{\partial T^n(\tilde{x}^{n-1}, \tilde{\theta}^n)}{\partial p^n} \tag{A.41}$$

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

and

$$\frac{\partial E^{n-1}}{\partial p^n} = \frac{\partial \tilde{x}^{n-1}}{\partial p^n} - \frac{\partial T^{n-1}(\tilde{x}^{n-2}, \tilde{\theta}^{n-1})}{\partial p^n} = \frac{\partial \tilde{x}^{n-1}}{\partial p^n} \tag{A.42}$$

$$n = 2, 3, \ldots, N.$$

By using the definition of Q^n, equation (A.20), the elements of equations (A.40), (A.41), and (A.42) become

$$\frac{\partial E_k^n}{\partial p_i^{n-1}} = - \left\{ \frac{\partial T_k^n}{\partial Q^n} \right\}^T \left\{ \frac{\partial Q^n}{\partial p_i^{n-1}} \right\} \tag{A.43}$$

$$k = 1, 2, \ldots, s^n$$

$$i = 1, 2, \ldots, s^{n-1}$$

$$n = 2, 3, \ldots, N,$$

$$\frac{\partial E_k^n}{\partial p_i^n} = \left\{D^{w^n+k}\right\}^T \left\{\frac{\partial Q^{n+1}}{\partial p_i^n}\right\} - \left\{\frac{\partial T_k^n}{\partial Q^n}\right\} \left\{\frac{\partial Q^n}{\partial p_i^n}\right\} \tag{A.44}$$

$k = 1, 2, \ldots, s^n$

$i = 1, 2, \ldots, s^n$

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

and

$$\frac{\partial E_k^{n-1}}{\partial p_i^n} = \left\{D^{w^n+k}\right\}^T \left\{\frac{\partial Q^n}{\partial p_i^n}\right\} \tag{A.45}$$

$k = 1, 2, \ldots, s^{n-1}$

$i = 1, 2, \ldots, s^n$

$n = 2, 3, \ldots, N.$

Substituting equations (A.37) and (A.38) into equations (A.43, (A.44), and (A.45), we obtain

$$\frac{\partial E_k^n}{\partial p_i^{n-1}} = -\left\{\frac{\partial T_k^n}{\partial Q^n}\right\}^T (B^n)^{-1} \left\{D^{w^n+i}\right\}$$

$$+ \left\{\frac{\partial T_k^n}{\partial Q^n}\right\}^T (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T (C^n)^{-1} \left\{F_i^n\right\} \tag{A.46}$$

$k = 1, 2, \ldots, s^n$

$i = 1, 2, \ldots, s^{n-1}$

$k = 2, 3, \ldots, N$

$$\frac{\partial E_k^n}{\partial p_i^n} = \left\{D^{w^n+k}\right\}^T (B^{n+1})^{-1} \left\{D^{w^{n+1}+i}\right\}$$

$$- \left\{D^{w^n+k}\right\}^T (B^{n+1})^{-1} \left(\frac{\partial R^{n+1}}{\partial Q^{n+1}}\right)^T (C^{n+1})^{-1} \left\{F_i^{n+1}\right\}$$

$$+ \left\{\frac{\partial T_k^n}{\partial Q^n}\right\}^T (B^n)^{-1} \left\{\frac{\partial T_i^n}{\partial Q^n}\right\}$$

$$- \left\{\frac{\partial T_k^n}{\partial Q^n}\right\}^T (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T (C^n)^{-1} \left\{G_i^n\right\} \qquad \text{(A.47)}$$

$k = 1, 2, \ldots, s^n$

$i = 1, 2, \ldots, s^n$

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

and

$$\frac{\partial E_k^{n-1}}{\partial p_i^n} = - \left\{D^{w^n+k}\right\}^T (B^n)^{-1} \left\{\frac{\partial T_i^n}{\partial Q^n}\right\}$$

$$+ \left\{D^{w^n+k}\right\}^T (B^n)^{-1} \left(\frac{\partial R^n}{\partial Q^n}\right)^T (C^n)^{-1} \left\{G_i^n\right\} \qquad \text{(A.48)}$$

$k = 1, 2, \ldots, s^{n-1}$

$i = 1, 2, \ldots, s^n$

$n = 2, 3, \ldots, N.$

By substituting the matrices C^n, G_i^n, and F_i^n into equations (A.46), (A.47), and (A.48), and noting that C^n and B^n are symmetric, it can be seen that

$$\frac{\partial E_k^n}{\partial p_i^{n-1}} = \frac{\partial E_i^n}{\partial p_k^{n-1}} \, , \quad \frac{\partial E_k^n}{\partial p_i^n} = \frac{\partial E_i^n}{\partial p_k^n} \, , \quad \frac{\partial E_i^{n-1}}{\partial p_i^n} = \frac{\partial E_i^{n-1}}{\partial p_k^n} \, ,$$

and

$$\left(\frac{\partial E^n}{\partial p^{n-1}}\right) = \left(\frac{\partial E^{n-1}}{\partial p^n}\right)^T .$$

That means that $\frac{\partial E_n}{\partial p^m}$ and $\frac{\partial E}{\partial p}$ are symmetric matrices. This enables us to consider the entire matrix of $\frac{\partial E}{\partial p}$ rather than just its symmetric part.

To prove that $\frac{\partial E}{\partial p}$ is negative definite, let us introduce a quadratic form defined as

$$\beta = \sum_{n=1}^{N} \{H^n\}^T (B^n)^{-1} \{H^n\} \tag{A.49}$$

where

$$H^n = B^n \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\} + B^n \frac{\partial Q^n}{\partial p^{n-1}} \{\lambda^{n-1}\} \tag{A.50}$$

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

and $\{\lambda^n\}$ is a column vector with elements of s^n arbitrary real numbers. When equations (A.49) and (A.50) are combined, the quadratic form becomes

$$\beta = \sum_{n=1}^{N} \left\{ \left(B^n \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\} + B^n \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}\right)^T (B^n)^{-1} \right.$$

$$\left. \cdot \left(B^n \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\} + B^n \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}\right)\right\}$$

$$= \sum_{n=1}^{N} \left\{ \{\lambda^n\}^T \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\} \right.$$

$$+ \{\lambda^{n-1}\}^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\}$$

$$+ \{\lambda^n\}^T \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}$$

$$\left. + \{\lambda^{n-1}\}^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\} \right\} . \tag{A.51}$$

Since (B) is a symmetric matrix and

$$\left\{\{\lambda^n\}^T \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}\right\}$$

is a scalar quantity, their transpose should be identical, that is

$$(B^n)^T = (B^n) \ ,$$

$$\left\{\{\lambda^n\}^T \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}\right\}^T$$

$$= \{\lambda^{n-1}\}^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\} \ . \tag{A.52}$$

Thus equation (A.51) becomes

$$\beta = \sum_{n=1}^{N} \left\{\{\lambda^n\}^T \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\}\right.$$

$$+ 2\{\lambda^{n-1}\}^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \{\lambda^n\}$$

$$\left. + \{\lambda^{n-1}\}^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \{\lambda^{n-1}\}\right\} \ . \tag{A.53}$$

This is a quadratic form of λ's, which can be written as

$$\beta = \{\lambda\}^T (A) \{\lambda\} \tag{A.54}$$

where

$$\{\lambda\}^T = (\{\lambda^1\}^T \{\lambda^2\}^T \ldots \{\lambda^N\}^T)$$

is a

$$\sum_{n=1}^{N} s^n$$

dimensional row vector.

We shall now prove that

$$(A) = \frac{\partial E}{\partial p} \quad . \tag{A.55}$$

Equation (A.55) will be proved if we can show that the coefficient of $\{\lambda^n\}^T \{\lambda^n\}$ in β is $\frac{\partial E^n}{\partial p^n}$ and the coefficient of $\{\lambda^n\}^T \{\lambda^{n-1}\}$ in β is $\frac{\partial E^n}{\partial p^{n-1}}$.

(a) Proof that the coefficient of $\{\lambda^n\}^T \{\lambda^{n-1}\}$ in β is equal to $\frac{\partial E^n}{\partial p^{n-1}}$. From equation (A.51), the coefficient of $\{\lambda^n\}^T \{\lambda^{n-1}\}$ term is

$$\left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) .$$

Taking the transpose of the equation (A.24) we have

$$\left\{(B^n) \left(\frac{\partial Q^n}{\partial p^n}\right)\right\}^T = \left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T$$

$$= - \left(\frac{\partial T^n}{\partial Q^n}\right) - \left(\frac{\partial u^n}{\partial p^n}\right) \left(\frac{\partial R^n}{\partial Q^n}\right) . \tag{A.56}$$

Postmultiplying equation (A.56) by

$$\left(\frac{\partial Q^n}{\partial p^{n-1}}\right)$$

we obtain

$$\left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^{n-1}}\right)$$

$$= - \left(\frac{\partial T^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) - \left(\frac{\partial u^n}{\partial p^n}\right)^T \left(\frac{\partial R^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \quad . \qquad (A.57)$$

When equation (A.27) is substituted into equation (A.57), we obtain

$$\left(\frac{\partial Q^n}{\partial p^{n-1}}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) = - \left(\frac{\partial T^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^{n-1}}\right) \quad . \qquad (A.58)$$

This equation is exactly the equation needed to complete the proof.

(b) Proof that the coefficient of $\{\lambda^n\}^T \{\lambda^n\}$ in β is equal to $\frac{\partial E^n}{\partial p^n}$.

From equation (A.51), the coefficient of $\{\lambda^n\}^T \{\lambda^n\}$ term is

$$\left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) \quad \text{and} \quad \left(\frac{\partial Q^{n+1}}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^{n+1}}{\partial p^n}\right) \quad .$$

By postmultiplying equation (A.56) by $\left(\frac{\partial Q^n}{\partial p^n}\right)$, we obtain

$$\left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right)$$

$$= - \left(\frac{\partial T^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^n}\right) - \left(\frac{\partial u^n}{\partial p^n}\right)^T \left(\frac{\partial R^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^n}\right) \quad . \qquad (A.59)$$

By using the condition, equation (A.25), equation (A.59) becomes

$$\left(\frac{\partial Q^n}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) = - \left(\frac{\partial T^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^n}\right) \quad . \qquad (A.60)$$

Taking the transpose of the equation (A.26), we obtain

$$\left(\frac{\partial Q^{n+1}}{\partial p^n}\right)^T (B^n)^T = (D)^T - \left(\frac{\partial u^{n+1}}{\partial p^n}\right)^T \left(\frac{\partial R^{n+1}}{\partial Q^{n+1}}\right) \tag{A.61}$$

where (D) is a (w^{n+1}+ s^n) by s^n matrix, with a s^n by s^n unit matrix I under a w^{n+1} by s^n null matrix.

Postmultiplying by $\left(\frac{\partial Q^{n+1}}{\partial p^n}\right)$, equation (A.61 becomes

$$\left(\frac{\partial Q^{n+1}}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^{n+1}}{\partial p^n}\right)$$

$$= (D)^T \left(\frac{\partial Q^{n+1}}{\partial p^n}\right) - \left(\frac{\partial u^{n+1}}{\partial p^n}\right)^T \left(\frac{\partial R^{n+1}}{\partial Q^{n+1}}\right) \left(\frac{\partial Q^{n+1}}{\partial p^n}\right) \quad . \tag{A.62}$$

By using the condition of equation (A.27), equation (A.62) becomes

$$\left(\frac{\partial Q^{n+1}}{\partial p^n}\right)^T (B^n)^T \left(\frac{\partial Q^n}{\partial p^n}\right) = (D)^T \left(\frac{\partial Q^{n+1}}{\partial p^n}\right) \quad . \tag{A.63}$$

Combining equations (A.60) and (A.63), the coefficient of $\{\lambda^n\}^\lambda$ $\{\lambda^n\}$ term is

$$(D)^T \left(\frac{\partial Q^{n+1}}{\partial p^n}\right) - \left(\frac{\partial T^n}{\partial Q^n}\right) \left(\frac{\partial Q^n}{\partial p^n}\right) \quad . \tag{A.64}$$

Comparison with equation (A.44) shows that this quantity is precisely $\frac{\partial E^n}{\partial p^n}$.

Thus equation (A.55) is proved. This means that $\frac{\partial E}{\partial p}$ is the matrice of the quadratic form β. But from the definition of β, equation (A.49), the quadratic form is a sum of smaller quadratic forms, $\{H^n\}^T$ $(B^n)^{-1}$ $\{H^n\}$. Thus we link the negative definiteness of $\frac{\partial E}{\partial p}$ with the negative definiteness of the matrices $(B^n)^{-1}$.

Since $(B^n)(B^n)^{-1} = (I)$, which is positive definite, the negative definiteness of the matrices (B^n) will guarantee the negative definiteness of the matrice, $(B^n)^{-1}$.

By the definition, equation (A.23), the matrices B^n are related to the matrices of second partial derivatives of the subobjective functions S^n and of the constraints R_i^n. The structure of the matrices B^n will, of course, vary with P, since which constraints are active and which are not depends upon P. This leads to the following theorem (6).

Theorem. If for all n, the subobjective function S^n and all the constraints R^n are concave (for maximization problems) in the arguments x^{n-1} and θ^n for all real values of P, and if at least one of these functions is strictly concave, the price-adjustment rule, equation (1.17), Chapter III, Part One, is asymptotically stable in the large, and convergence to $\overline{P}$ is monotone in $\|E\|$.

Proof. By the hypotheses, the matrices J^n and K_i^n in equations (A.21) and (A.22) are negative semidefinite, with at least one negative definite, for all P, θ^n, and x^{n-1}, $n = 1, 2, \ldots, N$, $i = 1, 2, \ldots, r^n$.

Then by equation (A.23) all B^n, and hence $(B^n)^{-1}$, are negative semidefinite, with at least one negative definite. This implies that in the expression, equation (A.49), the quadratic form β is negative definite for all λ and P, which guarantees the negative definite of the matrice $\dfrac{\partial E}{\partial p}$.

It is shown in section 2, Chapter III, Part One, that asymptotic stability in the large of price-adjustment rule, equation (1.17), Chapter III, Part One, requires that $\frac{dV}{dt}$ be negative definite for all P or, equivalently, that in the expression (1.20), Chapter III, Part One, $\frac{\partial E}{\partial p}$ should be negative definite for all P. Thus the proof is completed.

A COMPARATIVE STUDY OF THE MAXIMUM PRINCIPLE AND THE MULTI-LEVEL SYSTEM THEORY AND THEIR APPLICATION

by

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A comparative and critical study of the multi-level system theory and the maximum principle was carried out. While the two-level structure of the multi-level theory was proved to be identical to the discrete maximum principle for simple recycle processes, it appears to be extremely difficult, if not impossible, to equate the multi-level theory to the discrete maximum principle for systems which are more complex than the two-level structure. However, it is plausible that we can develop an optimization technique in which both the multi-level theory and the discrete maximum principle can be jointly used. In an attempt to develop such a method the maximum principle was extended to systems with inequality constraints by using the Kuhn and Tucker complementary slackness principle which is one of the tools employed in developing the multi-level theory. The system model and performance equations of the reverse-osmosis water purification process were developed for the purpose of optimizing the process by means of the multi-level approach and/or the discrete maximum principle.