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THE OPTIMIZATION OF A TUBULAR CHEMICAL REACTOR: A STUDY OF THE PSEUDO-OPTIMUM SEARCH METHOD

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THE OPTIMIZATION OF A TUBULAR CHEMICAL REACTOR:

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ABSTRACT

A pseudo-optimum search method is developed for studying multi-stage optimization problems. Other techniques, such as the maximum principle, dynamic programming, and search methods, including the steepest ascent methods and Newton's methods, have been applied for solving these types of problems. The applicability of the first two methods is restricted, and the convergence of these particular search methods is slow and uncertain. The proposed pseudo-optimum method was proved to be a powerful and elegant technique in the following optimization problems while other methods failed or were inadequate in their convergence rate.

The problems considered were:

(1) The optimal design of a tubular chemical reactor with radial gradients of concentration and temperature. Using this modified pseudo-optimum method, the optimal heat flux profile is obtained within a very few iterations and is shown to be a powerful convergence technique.

(2) The optimal temperature policy in a one-dimensional tubular reactor with a complicated reaction scheme.

(3) The optimal control of an absorption tower. Using the pseudo-optimum method, it is possible to manipulate the liquid flow rate for attaining a new steady state in a minimum amount of time.

The method is particularly applicable to problems involving stage-type calculations.

TABLE OF CONTENTS

		Page
LIST OF TABLES		viii
LIST OF ILLUSTRATIONS		ix
Chapter		
I.	INTRODUCTION	1
	1. Mayer's Problem	1
	2. Dynamic Programming	3
	3. The Maximum Principle	7
	4. The Gradient Method in Functional Space	12
II.	THE COMPARISON OF OPTIMAL SEARCH METHODS IN THE CASE OF A SIMPLIFIED REACTOR MODEL	18
	1. Analytic Solution of Optimal Temperature Profile	18
	2. Bryson's Application of the Gradient Method in Functional Space	25
	3. Newton's Method	39
	4. Other Methods	47
	5. Conclusion	55
III.	THE PSEUDO-OPTIMUM METHOD	59
	1. Development of the Method	59
	2. Numerical Example: Sequence of Stirred Tank Reactors	67
	3. Numerical Example: Absorption Tower	75
IV.	OPTIMIZATION OF A TWO-DIMENSIONAL TUBULAR REACTOR	85
	1. Previous Work	85
	2. Fixed Bed Reactor Model	91

TABLE OF CONTENTS (Continued)

Chapter		Page
	3. Optimal Heat Flux Profile: A Computation Strategy	99
	4. Results of Computation.	103
V.	CONCLUSION AND RECOMMENDATIONS FOR FURTHER WORK	122
BIBLIOGRAPHY		127
NOMENCLATURE		131
APPENDIX		136

LIST OF TABLES

Table		Page
1	Computation Parameters for a One-Dimensional Reactor.	24
2	First and Second Order Adjoints of Heat Flux	45
3	First and Second Order Adjoints of Heat Flux at Uniform Temperature Distribution .	46
4	The Results of Two Ascending Series	75
5	Parameter Values for Computation.	103
6	Initial and Final Conditions of First Ascent Series.	112
7	Initial and Final Conditions of Second Ascent Series.	113

LIST OF ILLUSTRATIONS

Figure		Page
1	The Dimensionless Heat Flux Profiles of Various Trials and Optimum ($\Phi = \infty$) for One-Dimensional Reactor Model.	28
2	The Dimensionless Temperature Profiles of Various Trials and Optimum for One-Dimensional Reactor Model.	29
3	The Dimensionless Concentration Profiles of Various Trials and Optimum for One-Dimensional Reactor Model.	30
4	Comparison of Dimensionless Heat Flux Difference Between the Initial Estimate and the Final Optimal One (ΔQ^*) and Dimensionless Heat Flux Adjusted in the First Trial (ΔQ)	31
5	The Profiles of Decision Variables, q, of Various Trials and Optimal Condition . . .	34
6	The Values of Profit Function of Consecutive Trials	35
7	Dimensionless Temperature Profiles of Consecutive Trials and Optimal Condition for One-Dimensionless Reactor Model.	48
8	Dimensionless Temperature Profiles of Consecutive Trials for One-Dimensional Reactor Model.	50
9	Dimensionless Temperature Profiles of Consecutive Trials and Optimal Condition for One-Dimensional Reactor Model	52
10	Reaction Rate Versus Temperature at Various Concentration.	53
11	$\frac{dR}{dT}$ Versus T at Various Concentrations	54

LIST OF ILLUSTRATIONS (Continued)

Figure		Page
12	Dimensionless Temperature Profiles of Consecutive Trials for One-Dimensional Reactor Model	56
13	Dimensionless Temperature Profiles of Consecutive Trials for One-Dimensional Reactor Model	57
14	Flow Chart of One-Dimensional Search. . . .	71
15	Flow Chart for Evaluating Profit for a Given Set of Decisions	72
16	Successive Approximation to Three Stage Temperature Policy	73
17	Iteration Trajectories of Concentration a_3 and b_3.	74
18	Discrete Optimal Liquid Flow Rate L' Versus Time for a Maximum Allowable Variation of 20%	81
19	Discrete Optimal Liquid Flow Rate L' Versus Time for a Maximum Allowable Variation of 40%	82
20	Discrete Optimal Liquid Flow Rate L' Versus Time for a Maximum Allowable Variation of 100%.	83
21	The Transient Response of Outlet Liquid Concentration, x_6, for Six Tray Absorption Column.	84
22	Two-Dimensional Reactor, Showing How Mixing Mechanism Occurs.	93
23	Comparison of Concentration Calculated Using Different Grid Sizes for Two-Dimensional Reactor Model.	105
24	Comparison of Temperature Calculated Using Different Grid Sizes for Two-Dimensional Reactor Model.	106
25	Flow Chart of Computational Procedure of a Single Stage in Two-Dimensional Reactor Model.	108

LIST OF ILLUSTRATIONS (Continued)

Figure		Page
26	Cross-Sectional Average Temperature Profiles Consecutive Trials: Ascending Series-A.	110
27	Cross-Sectional Average Temperature Profiles Consecutive Trials: Ascending Series-B.	111
28	Initial and Optimal Temperature Profiles For Two-Dimensional Reactor Model. . . .	114
29	Initial and Optimal Concentration Profiles For Two-Dimensional Reactor Model. . . .	115
30	Initial and Optimal Heat Flux Profiles For Two-Dimensional Reactor Model.	116
31	Pseudo-Optimum Temperature Difference of Wall Stage. Consecutive Trials: Ascending Series-A	117
32	Pseudo-Optimum Temperature Difference of Wall Stage. Consecutive Trials: Ascending Series-B	118
33	Comparison of the Yields of Three-Ascending Convergence Series. Two-Dimensional Reactor Model.	119
34	Gradient in Functional Space of Two-Dimensional Reactor Model. Consecutive Trial: Ascending Series-C	120
35	Comparison of Final Temperature Distributions Calculated by the Pseudo-Optimum Method and the Gradient Method	121

THE OPTIMIZATION OF A TUBULAR CHEMICAL REACTOR: A STUDY OF THE PSEUDO-OPTIMUM SEARCH METHOD

CHAPTER I

INTRODUCTION

1. Mayer's Problem

Consider a Mayer's problem, [D.5] which usually appears in the following form:*

$$\frac{d\,x_s}{d\,z} = f_s(x_1, \ldots, x_S, z, q) \quad \text{for } s = 1, \ldots, S. \qquad (1.1\text{-}1)$$

where x_s is a state variable, z is the independent variable, and q is the control function. The initial conditions specified at time z_o are

$$x_s(z_o) = x_s^o \qquad \text{for } s = 1, \ldots, S$$

The problem is to find a control function, q(z), which yields a state trajectory

$$x_s(z) \text{ from } z = z_o \text{ to } z = \theta, \text{ for } s = 1, \ldots, S.$$

---

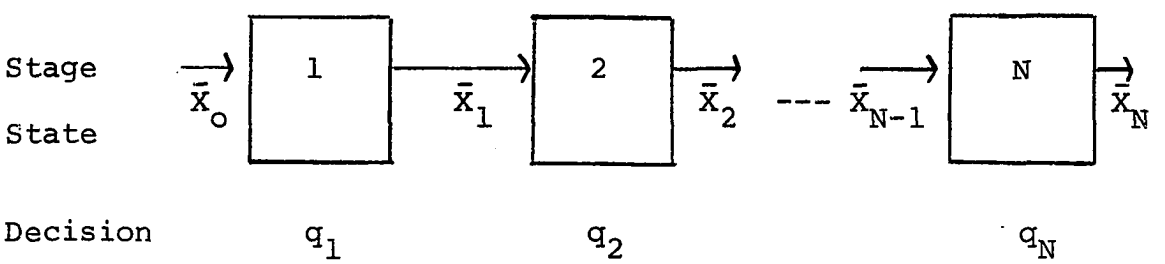
*A list of notations is given in the appendix.

with the property that at the terminal time $z = \theta$, the object function

$$Y(x_1(\theta), \ldots, x_S(\theta), \theta)$$

attains its maximum or minimum value.

In a discrete case, this problem is called a multistage decision process. It can be represented by the following diagram



where

$$\bar{X}_i = \bar{F}_i(\bar{X}_{i-1}, q_i) \quad \text{for } i = 1, \ldots, N \qquad (1.1\text{-}2)$$

The problem is to find a sequence of control variables (or vectors) $q_1, \ldots, q_N$, which will give the maximum or minimum of an object function, $Y(\bar{X}_N)$.

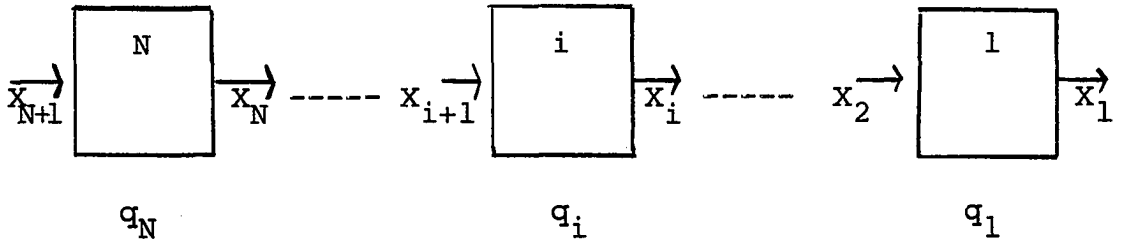
The maximum principle, dynamic programming, and optimum search methods have been applied to solving these types of problems. However, the applicability of the first two methods is restricted, and the convergence of search methods is usually slow and uncertain. These methods will be reviewed in the following sections.

2. Dynamic Programming

Dynamic programming has become well known to chemical engineers, since Bellman [B.1] developed it in 1957. This technique is based on the principle of optimality, which states:

> An optimal policy has the property that whatever the initial state and initial decisions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision.

Consider the multistage decision process problem illustrated in the following diagram



where i is the number of stages as numbered from the end $\bar{X}_{i+1}$ and $\bar{X}_i$ are the feed and the product state vectors respectively, q_i is the operating state (decision), and y_i is the net profit from the i-th stage. The transformation equations are

$$\bar{X}_i = \bar{F}_i(\bar{X}_{i+1} ; q_i) \qquad (1.2\text{-}1)$$

$$y_i = y_i(\bar{X}_{i+1} ; q_i) \qquad (1.2\text{-}2)$$

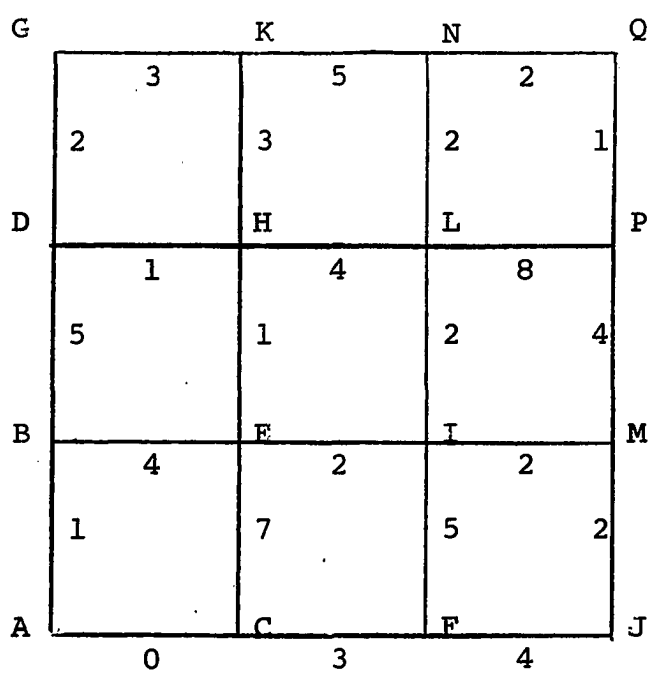
An object function can be defined by

$$f_N(\bar{X}_{N+1}) = \text{Max} \sum_{1}^{N} y_i(\bar{X}_{i+1} \; ; \; q_i), \qquad (1.2\text{-}3)$$

The principle of optimality when applied to the above system gives

$$f_N(X_{N+1}) = \underset{q_N}{\text{Max}} \; [y_N + f_{N-1}(X_N)] \qquad (1.2\text{-}4)$$

To demonstrate the application of dynamic programming, a simple example is given. The problem is to choose a path or procedure to go from point A to point Q, which will make the most profit.



The numbers in the diagram indicate the net profit between two points. We also assume that the routine may only advance

either upward or rightward. Define f(X) to be the value of maximum profit from a point X to the final point Q. By the principle of optimality, we have

$$f(Q) = 0$$

$$f(N) = y_{NQ} = 2$$

$$f(P) = y_{PQ} = 1$$

$$f(L) = \text{Max}\begin{pmatrix} y_{LP} + f(P) \\ y_{LN} + f(N) \end{pmatrix} = \text{Max } (9 \; ; \; 4) = 9$$

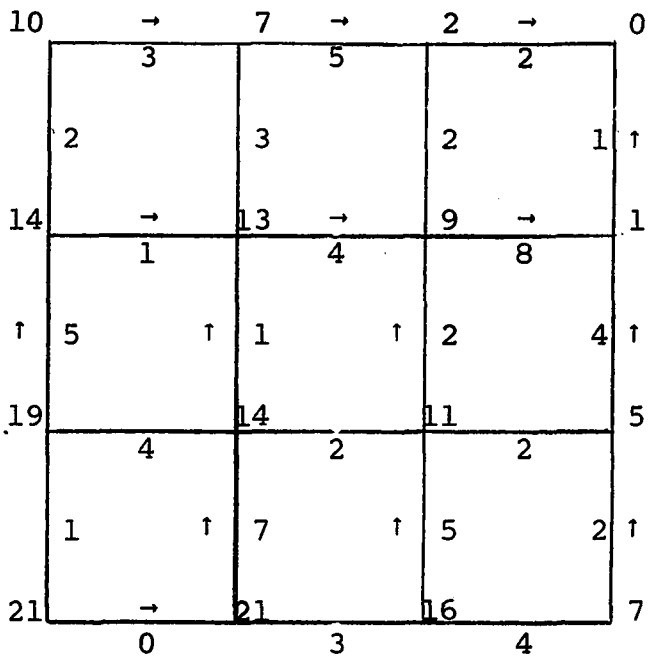
.....

$$f(A) = \text{Max}\begin{pmatrix} y_{AB} + f(B) \\ y_{AC} + f(C) \end{pmatrix} = \text{Max } (20 \; ; \; 21) = 21$$

Where y is the net profit between points. The actual values of the object function and decisions are shown in the following diagram.

However, this example is an over simplified problem. Most problems in chemical engineering differ from this example by the following two characteristics: (1) the final state is not specified, (2) the decision in each stage is a continuous function. Consider, for example, the problem of finding an optimal temperature distribution which will give maximum yield in a series of

stirred tank reactors. Because of the above two difficulties, dynamic programming is used as a basis of analytic solution rather than a direct tabular computing procedure. Even so, the direct analytic equations are still unsolvable, except for a few simple problems.



Pismen and Ioffe [P.1] suggested an alternative method of solution; let the backward transformation function and the profit function be

$$\left.\begin{aligned} \bar{X}_{i+1} &= \bar{F}_i(\bar{X}_i \; ; \; q_i) \\ y_i &= y_i(\bar{X}_i \; ; \; q_i) \end{aligned}\right\} \text{for } i = 1, \ldots, N$$

Their computing procedure is as follows:

1. Estimate the values of state variables at final condition, $\bar{X}_1$.

2. By the principle of optimality, we have

$$f_2(\bar{X}_2) = \underset{q_1}{\text{Max}} \; [y_1(\bar{X}_1 \; ; \; q_1)]$$

Solve for q_1, then by the transformation equation we have

$$\bar{X}_2 = \bar{F}_1(\bar{X}_1 \; ; \; q_1)$$

3. Solve q_2 from

$$f_3(\bar{X}_3) = \underset{q_2}{\text{Max}} \; [y_2(\bar{X}_2 \; ; \; q_2) + f_2(\bar{X}_2)]$$

then

$$\bar{X}_3 = \bar{F}_2(\bar{X}_2 \; ; \; q_2)$$

and so on until the input condition is reached. In general, the computed value of X_{N+1} will not agree with the given initial condition.

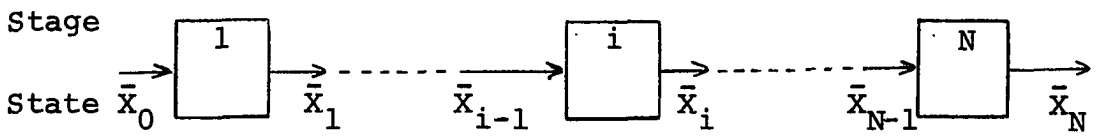
4. Re-estimate the final state and repeat the cycle.

There is no reason to expect that this approach will converge and even if it does it will usually require excessive computer time.

3. The Maximum Principle

The maximum principle was first derived by Pontryagin [P.2], Chang [C.3, C.4] and Katz [K.1] extended the results to discrete multistage decision processes.

Consider a process shown in the following diagram



The state vector $\bar{X}_i$ is related to the previous state and the decision, q_i, by

$$\bar{X}_i = \bar{F}_i(\bar{X}_{i-1} ; q_i) \quad \text{for } i = 1, \ldots, N \qquad (1.3\text{-}1)$$

and the object function to be maximized is $Y(\bar{X}_N)$. Introduce the Hamiltonian

$$H_i = \sum_{s=1}^{S} z_i^s x_i^s \qquad (1.3\text{-}2)$$

where x_i^s denotes a component of the vector $\bar{X}_i$. z_i^s, a component of Green's vector, is defined as

$$z_{i-1}^s = \sum_{s'=1}^{S} \frac{\partial F_i^{s'}}{\partial x_{i-1}^s} z_i^{s'} \quad \text{for } s = 1, \ldots, S \qquad (1.3\text{-}3)$$

with the boundary condition

$$z_N^s = \frac{\partial Y(\bar{X}_N)}{\partial x_N^s} \qquad s = 1, \ldots, S \qquad (1.3\text{-}4)$$

Then the following relation can be obtained by using Green's identity:

$$z_N^s \, \delta x_N^s = z_o^s \, \delta x_o^s + \sum_{i=1}^{N} z_i^s \frac{\partial T_i^s}{\partial q_i} \, \delta q_i \qquad (1.3\text{-}5)$$

Since

$$\frac{\partial H_i}{\partial q_i} = \sum_{s=1}^{S} z_i^s \frac{\partial x_i^s}{\partial q_i} = \sum_{s=1}^{S} z_i^s \frac{\partial F_i^s}{\partial q_i} \qquad (1.3\text{-}6)$$

equation (1.3-5) can be written as

$$\sum_{s=1}^{S} z_N^s \, \delta x_N^s = \sum_{s=1}^{S} z_o^s \, \delta x_o^s + \sum_{i=1}^{N} \frac{\partial H_i}{\partial q_i} \, \delta q_i \qquad (1.3\text{-}7)$$

A perturbation in the object function can be expressed as

$$\delta Y = \sum_{s=1}^{S} \frac{\partial Y}{\partial x_N^s} \, \delta x_N^s \qquad (1.3\text{-}8)$$

Substitute equation (1.3-8) into the left-hand side of equation (1.3-7).

$$\delta Y = \sum_{s=1}^{S} z_o^s \, \delta x_o^s + \sum_{i=1}^{N} \frac{\partial H_i}{\partial q_i} \, \delta q_i \qquad (1.3\text{-}9)$$

If the initial conditions are considered to be fixed, then equation (1.3-9) reduces to

$$\delta Y = \sum_{i=1}^{N} \frac{\partial H_i}{\partial q_i} \, \delta q_i \qquad (1.3\text{-}10)$$

It is quite obvious that the necessary and sufficient condition for $\delta Y = 0$ is

$$\frac{\partial H_i}{\partial q_i} = 0 \qquad \text{for } i = 1, \ldots, N \qquad (1.3\text{-}11)$$

This result is the necessary condition of optimization in a multistage decision process.

Fan [F.1] argued that there is a difference between equation (1.3-11) and (1.3-12) H_i = Maximum, for i = 1, ..., N. For a linear transformation function, equation (1.3-12) provides the sufficient as well as necessary conditions for optimum, but equation (1.3-11) does not. However, for the general case, neither set of equations is sufficient for attaining the optimum.

Except for quite simple problems, the set of N equations is very difficult or impossible to solve.

Katz suggested the following iteration scheme

1. Guess a sequence of values for $q_1, \ldots\ldots q_N$.
2. Solve the state trajectory described by equation (1.3-1) forward from i = 1 to i = N.
3. Based on these states, solve the adjoint equation (1.3-3) and (1.3-4) backward from i = N to i = 1.
4. With these $\bar{X}$'s and z's compute a new sequence of q's from (1.3-10), and return to step 2.

Denn and Aris [D.3] proposed two other computational schemes. The first scheme involves the assumption of a

set of values at the final point and then carrying out the maximization of the Hamiltonian backward to the initial point. In general, the calculated initial conditions do not correspond to the given initial conditions. Improved values at final point were given by

$$x_N^s|_{New} = x_N^s|_{Old} + \sum_{k=1}^{S} z_{ok}^s \left(x_o^k|_{given} - x_o^k|_{calculated}\right)$$

where z is Green's tensor, defined by equation (1.3-3), with the boundary condition

$$z_{N,k}^s = \delta_k^s \qquad \text{for } s = 1, \ldots, S,\ k = 1, \ldots, S$$

$$S_k^s = \begin{cases} 1, & \text{for } s = k \\ 0, & \text{for } s \neq k \end{cases}$$

Then this routine is iterated until the calculated initial conditions agree with the given conditions. However, two assumptions were made for the above equation. They are (1) the values of sequence $q_1, \ldots\ldots q_N$ do not change during consecutive trials. (2) second and higher derivative terms of Taylor's expansion are neglected. Therefore, the converging rate of this scheme depends on how good these assumptions are.

The second technique described by Denn and Aris [D.3] is to use the gradient of the Hamiltonian with respect to the decision for the steepest ascent direction.

This scheme is similar to the one derived by Bryson and Denham [B.2], which is reviewed in the next section.

4. The Gradient Method in Functional Space

Due to the availability of high speed computers in recent years, Bryson and Denham [B.2] applied the steepest ascent method to solving Mayor's problem. Their computation procedure is summarized as follows:

1. Estimate a reasonable control function, $q(z)$. Then evaluate the state trajectory and the terminal object function.

2. Consider the control function, $q(z)$, to be perturbed by $\delta q(z)$, which will cause a perturbation in the state trajectory

$$\delta x_s(z) \quad \text{for } s = 1, \ldots, S$$

Suppose $\delta q(z)$ is small enough to allow the first order expansion about $\delta x_s(z)$ and $\delta q(z)$, then equation (1.1-1) becomes

$$\frac{d}{dz}(\delta x_s) = \frac{\partial f_s}{\partial x_1}\delta x_1 + \ldots + \frac{\partial f_s}{\partial x_S}\delta x_S + \frac{\partial f_s}{\partial q}\delta q(z) \quad (1.4\text{-}1)$$

$$\text{for } s = 1, 2, \ldots, S$$

Written in matrix form, (1.4-1) becomes

$$\frac{d}{dz}(\delta\bar{X}) = \bar{\bar{F}}(z)\cdot\delta\bar{X} + \bar{G}(z)\,\delta q(z) \quad (1.4\text{-}2)$$

where

$$\bar{\bar{F}}(z) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_S} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_S}{\partial x_1} & \cdots & \frac{\partial f_S}{\partial x_S} \end{bmatrix} \quad \bar{G}(z) = \begin{bmatrix} \frac{\partial f_1}{\partial q} \\ \vdots \\ \frac{\partial f_S}{\partial q} \end{bmatrix} \tag{1.4-2A}$$

To obtain the solution, adjoint matrix $\bar{D}$ is introduced as follows

$$\frac{d\bar{D}}{dz} = - \bar{\bar{F}}^T(z) \cdot \bar{D} \tag{1.4-3}$$

where double bar means matrix, single bar means column matrix, and the superscript T denotes the transpose of the matrix. If we premultiply equation (1.4-2) by $\bar{D}^T$ and equation (1.4-3) by $\bar{X}^T$, we have

$$\sum_{s=1}^{S} D_s \frac{d(\delta x_s)}{dz} = \sum_{s=1}^{S} \left[\left(\frac{\partial f_s}{\partial x_1} \delta x_1 + \ldots + \frac{\partial f_s}{\partial x_S} \delta x_S + \frac{\partial f_s}{\partial q} \delta q \right) D_s \right] \tag{1.4-4}$$

$$\sum_{s=1}^{S} \delta x_s \frac{dD_s}{dz} = - \sum_{s=1}^{S} \left(\frac{\partial f_1}{\partial x_s} D_1 + \ldots + \frac{\partial f_S}{\partial x_s} D_S \right) \delta x_s \tag{1.4-5}$$

Adding equation (1.4-4) to equation (1.4-5), we obtain

$$\sum_{s=1}^{S} \left(D_s \frac{d(\delta x_s)}{dz} + \delta x_s \frac{dD_s}{dz} \right) = \sum_{s=1}^{S} \left(\frac{\partial f_s}{\partial q} \delta q \, D_s \right) \tag{1.4-6}$$

In matrix form

$$\frac{d}{dz}\left(\bar{D}^T \cdot \delta\bar{X}\right) = \bar{D}^T \cdot \bar{G}\,\delta q \qquad (1.4\text{-}7)$$

Integrating equation (1.4-7) between the limits 0 and θ, we have

$$\bar{D}^T \cdot \delta\bar{X}\Big|_0^\theta = \int_0^\theta \bar{D}^T \cdot \bar{G}\,\delta q\,dz \qquad (1.4\text{-}8)$$

where $\bar{D}$ was defined in the differential matrix equation (1.4-3). The boundary conditions can be specified as

$$\bar{D}\,(\theta) = \left(\frac{\partial Y}{\partial \bar{X}}\right)_{z=\theta} \qquad (1.4\text{-}9)$$

where Y is the object function. Substituting this relation into equation (1.4-8), we have

$$\delta Y = \int_0^\theta \bar{D}^T(z) \cdot \bar{G}\,\delta q\,dz + \bar{D}^T(o) \cdot \delta\bar{X}(0) \qquad (1.4\text{-}10)$$

If we consider the initial condition to be fixed, then

$$\delta Y = \int_0^\theta \bar{D}^T(z) \cdot \bar{G}\,\delta q\,dz \qquad (1.4\text{-}10A)$$

Actually, this assumption does not lose its generality, because the change of initial condition might be considered as a part of the control function. Let the total perturbation of q(z) be measured by

$$P = \int_0^{\theta} \delta^2 q(z)dz \qquad (1.4\text{-}11)$$

Using the LaGrange multiplier technique, we have

$$\mu P - \mu \int_0^{\theta} \delta^2 q(z)dz = 0 \qquad (1.4\text{-}11A)$$

Adding equation (1.4-11A) to equation (1.4-10A), we obtain

$$\delta Y = \int_0^{\theta} [\bar{D}^T \cdot \bar{G} - \mu\, \delta q(z)]\, \delta q(z)dz + \mu P \qquad (1.4\text{-}12)$$

where $\delta q(z)$ is a perturbation function, not specified yet. The maximum of Y can be obtained by differentiating equation (1.4-12) with respect to $\delta q(z)$

$$\bar{D}^T \cdot \bar{G} - 2\mu\delta q(z) = 0 \qquad (1.4\text{-}13)$$

So that

$$\delta q(z) = \frac{\bar{D}^T \cdot \bar{G}}{2\mu} = \frac{1}{2\mu} \sum_{s=1}^{S} D_s(z) \frac{\partial x_s}{\partial q}(z) \qquad (1.4\text{-}14)$$

Solving for μ from equations (1.4-11), (1.4-12) and (1.4-14) we obtain

$$\mu = \frac{1}{2} ,$$

and

$$\delta q(z) = \sum_{s=1}^{S} D_s(z) \frac{\partial x_s}{\partial q}(z) \qquad (1.4\text{-}15)$$

Using the optimal $\delta q(z)$, the maximum change of the object function is

$$\delta Y = \int_0^\theta \delta^2 q(z)dz = P \qquad (1.4\text{-}16)$$

If the integral $\int_0^\theta \bar{D}^T \cdot \bar{G}\, \delta q(z)dz$ is approximated by the summation of N equally divided sections, then

$$\delta Y = \int_0^\theta \bar{D}^T \cdot \bar{G}\, \delta q(z)dz = \sum_{i=1}^{N} \bar{D}^T \cdot \bar{G}\, \delta q_i \Delta z$$

where $N\ \Delta\ z = \theta$, and δq_i is the average value of $q(z)$ between $z = z_i - \frac{1}{2}\Delta z$ and $z = z_i + \frac{1}{2}\Delta z$. Because each section of $q(z)$ is an independent variable, so that

$$\frac{\partial Y}{\partial (q_i \Delta z)} \simeq \bar{D}^T \cdot \bar{G} = \sum_{s=1}^{S} D_s \frac{\partial x_s}{\partial q_i}$$

where D_s and x_s are evaluated at $z = z_i$. Also by equation (1.4-15), the optimal change of $q(z)$ over the range $z = z_i - \frac{1}{2}\Delta z$ to $z = z_i + \frac{1}{2}\Delta z$ should be

$$\delta q_i = \sum_{s=1}^{S} D_s(z_i) \frac{\partial x_s}{\partial q_i}$$

Therefore, the optimal change of $q(z_i)$ is proportional to the derivative of the object function with respect to $(q_i\ \Delta\ z)$.

Lee [L.4] first applied this technique to find the optimal temperature profile in a one-dimensional tubular

reactor for the reaction sequence A → B → C. He claimed that in comparison with solutions of other methods, good results were obtained after forty-five iterations. However, the initial condition was quite good and the reliability of this method was not tested by starting from different initial estimations.

Storey [S.2] also discussed the possibility of applying this method to obtain the optimal temperature policy in a tubular vessel for the reaction

$$\begin{array}{ccccccc} A & \rightarrow & B & \rightarrow & C & \rightarrow & D \\ & \swarrow & \searrow & & & & \\ D & & P & & & & \end{array}$$

where C is desired product. The rate of convergence and the instability depend on the step of ascent. After a certain number of iterations no improvement could be achieved, no matter how small the step is chosen. Storey also showed that the direction of the steepest ascent does not lead in the direction of the summit.

Gray [G.1, G.2] used the same method to seek the optimal heat flux profile for a reversible reaction in a two dimensional tubular reactor. However, he failed to achieve the same goal from different initial estimations.

CHAPTER II

THE COMPARISON OF OPTIMUM SEARCH METHODS IN THE CASE OF A SIMPLIFIED REACTOR MODEL

As seen in the last chapter even though the maximum principle and dynamic programming give the necessary conditions for an optimal solution, neither method provides sufficient strategy or power for solving optimization problems except for very simple cases. In general optimum seeking methods are more practical than the maximum principle and dynamic programming. However, the convergence of these various search methods is uncertain and cannot be predicted in advance for nonlinear systems.

In order to compare the convergence of search methods and to recommend a suitable technique for finding the optimal solution of complicated problems, various methods were tried for the solution of the simplified one-dimensional reactor with a first order reversible reaction. The solution of this problem can be obtained analytically and then used as a basis for comparison for the various methods.

1. Analytic Solution of Optimal Temperature Profile

By assuming the absence of radial gradient of heat, mass and momentum, the partial differential equation of a

tubular chemical reactor can be written as

$$- u \frac{\partial C}{\partial Z} + D_z \frac{\partial^2 C}{\partial Z^2} + r(C, T) = \frac{\partial C}{\partial t} \qquad (2.1\text{-}1)$$

At steady state, equation (2.1-1) can be written in dimensionless form

$$\frac{d^2 c}{dz^2} - \frac{dc}{dz} + \frac{D_z}{C_{in} u^2} r = 0 \qquad (2.1\text{-}2)$$

where the variables are defined

$$c = \frac{C}{C_{in}} \, , z = Zu/D_z$$

Letting the derivatives be represented by a standard central difference formula, (2.1-2) will appear in the form:

$$\frac{1}{\Delta z^2} [c_{i+1} - 2 c_i + c_{i-1}] - \frac{1}{2\Delta z} (c_{i+1} - c_{i-1}) + \frac{D_z}{C_{in} u^2} r = 0 \qquad (2.1\text{-}3)$$

where

$$\Delta z^2 = \frac{\Delta Z u}{D_z} = \frac{Lu}{D_z N}$$

L is the length of the reactor. N, an arbitrary but reasonably large number, represents the number of sections that the reactor is divided into. If we choose $\Delta z = 2$, then N can be calculated as $N = \frac{Lu}{2D_z}$. Substituting Δz into equation (2.1-3) yields

$$c_{i-1} - c_i + \frac{2D_z}{c_{in}u^2} r_i = 0 \qquad (2.1\text{-}4)$$

Defining

$$R_i = \frac{2D_z}{c_{in}u^2} r_i$$

then

$$c_i = c_{i-1} + R_i \qquad \text{for } i = 1, \ldots, N \qquad (2.1\text{-}5)$$

The distribution of temperatures can be derived in a similar way with the result

$$T_i = T_{i-1} + \lambda R_i - Q_i \qquad (2.1\text{-}6)$$

where

$$Q_i = \frac{\text{Heat removed at wall per unit time}}{\text{Enthalpy entering the section per unit time}}$$

$$= \frac{2\pi R_t \, \Delta z \, q(z_i)}{\pi R_t^2 \, \rho C_p \, T_{in} \, u} = \frac{2 \, L \, q(z_i)}{\rho \, C_p \, T_{in} \, u \, R_t} \, \frac{1}{N} \qquad (2.1\text{-}7)$$

ΔH = Enthalpy change per mole of reaction, Btu/mole

$q(z_i)$ = Heat flux, Btu/sq. ft.

R_t = Inside radius of reactor.

Summing up the equations (2.1-5) for stage 1 to stage N, we have

$$c_N - c_0 = \sum_{1}^{N} (c_i - c_{i-1}) = \sum_{1}^{N} R_i \qquad (2.1\text{-}8)$$

Also, define an objective function as

$$f_i(c_i) = \text{Max} \left(\sum_{j=i}^{N} R_j\right) = \text{Max} \ (c_N - c_i) \qquad (2.1\text{-}9)$$

By the principle of optimality, which states that "An optimal policy has the property that whatever the initial state and initial decisions are, the remaining decision must constitute an optimal policy with respect to the state resulting from the first decision," the following relation may be written

$$f_0(c_0) = \text{Max} \ [c_1 - c_0 + f_1(c_1)] \qquad (2.1\text{-}10)$$

If $f_1 \ (c_1)$ is represented by

$$f_1(c_1) = (1 - c_1) \ \eta_1 \qquad (2.1\text{-}11)$$

where $(1 - c_1)$ is the reactant concentration at the first stage and η is the maximum percentage conversion, [for example $c_1 = 0.2$ and Max $(c_N) = 0.8$

then $\eta_1 = \dfrac{0.8 - 0.2}{1.0 - 0.2} = 75\%$]

In general, the conversion will not be complete, therefore η_1 will be less than one. Then

$$\frac{d}{dc_1}\left[c_1 + f_1(c_1)\right]$$

$$= \frac{d}{dc_1}\left[c_1 + (1 - c_1)\eta_1\right]$$

$$= 1 - \eta_1 > 0 \qquad (2.1\text{-}12)$$

The positive derivative means that the increasing amount of c_1 will always favor the total conversion. Since c_1 is a function of T_1, T_1 should be chosen to maximize c_1, which is equivalent to maximizing R_1.

For a reversible reaction with the rate given as

$$R = \frac{D_{aI}}{N}\left[(1 - c)e^{E_1(1 - 1/T)} - c\, e^{E_{02} - E_2/T}\right] \qquad (2.1\text{-}13)$$

the optimal temperature will be

$$T_{opt} = \frac{E_2 - E_1}{E_{02} - E_1 - \ln\left(\frac{1 - c}{c}\frac{E_1}{E_2}\right)} \qquad (2.1\text{-}14)$$

For a general stage — i, the relation exists

$$f_{i-1}(c_{i-1}) = \text{Max}\left[c_i - c_{i-1} + f_i(c_i)\right]$$

where

$$f_i(c_i) = (1 - c_i)\eta_i$$

and $\eta_i < 1$

So that $\frac{d}{dc_i}\left[c_i - c_{i-1} + f_i(c_i)\right] = 1 - \eta_i > 0$

This implies that the objective function, $f_{i=1}(c_{i=1})$, is a function of the maximum of c_i. Therefore each stage temperature, T_i, should be chosen to maximize the reaction rate in its corresponding stage. From this, the optimal temperature is seen to be a function of local stage concentrations only, regardless of the decisions and states elsewhere. This decoupling of the system is called the disjoint property. However for two consecutive reactions or two simultaneous reactions, this disjoint property will not exist and therefore the solution will be much more complex.

The procedure for evaluating the optimal temperature concentration and heat flux in i-th stage is given as follows:

1. Estimate $c_i = c_{i-1}$

2. Evaluate the stage temperature from

$$T_i = \frac{E_2 - E_1}{E_{02} - E_1 - \ln\left(\frac{1 - c_i}{c_i}\frac{E_1}{E_2}\right)}$$

3. From the concentration and temperature obtained above, calculate the reaction rate by the following

$$R_i = \frac{Da_I}{N}\left[(1 - c_i)\, e^{E_1 - E_1/T_i} - c_i\, e^{E_{02} - E_2/T_i}\right]$$

4. Substitute $c_i = c_{i-1} + R_i$

5. Repeat step 2 through step 4, until the difference between two consecutive values of R_i is less than an assumed tolerable error.

6. Evaluate Q_i by

$$Q_i = T_{i-1} - T_i + \lambda R_i$$

7. Go to next stage.

To determine the parameters in the above equations, the numerical values as shown in Table 1 were chosen.

TABLE 1

COMPUTATION PARAMETERS FOR A ONE-DIMENSIONAL REACTOR

Dimensionless input temperature, T_o	1.0
Dimensionless input concentration, c_o	0.0382
$\lambda = \frac{\Delta H}{\rho C_p T_{in}}$	2.0
Axial length, L	4.524 ft.
Particle diameter, D_p	0.03 ft.
Number of stages, N	112
Kinetic constants, Da_I	0.2262
E_1	19.35
E_2	41.35
E_{02}	40.35

2. Bryson's Application of the Gradient Method in Functional Space

Gray [G.1, G.2] used this ascending method to search for an optimal heat flux of a two-dimensional reactor model. To determine the efficiency of this method and the reliability of Gray's result, this technique was applied to the search for an optimal heat flux profile for a simplified model. The analytic solution obtained in the last section provides a basis for comparison. The computational procedure for this method is summarized as follows:

1. Estimate a reasonable heat flux profile Q(z) and calculate the concentration and temperature along the reactor.
2. Integrate the following adjoint equations from z = 1 to z = 0.

$$\frac{dD_C}{dz} = - \left(\frac{\partial R}{\partial c} D_C + \lambda \frac{\partial R}{\partial c} D_T \right) \qquad (2.2\text{-}1)$$

$$\frac{dD_T}{dz} = - \left(\frac{\partial R}{\partial T} D_C + \lambda \frac{\partial R}{\partial T} D_T \right) \qquad (2.2\text{-}2)$$

with the boundary conditions

$$D_C(z) = 1 \text{ and } D_T(z) = 0 \text{ , at } z = 1 \qquad (2.2\text{-}3)$$

Expressing in finite difference form, these equations are

$$D_C|_i = D_C|_{i+1} - \frac{\partial R}{\partial c}\Big|_i \cdot D_C|_{i+1} - \lambda \frac{\partial R}{\partial c}\Big|_i \cdot D_T|_{i+1} \qquad (2.2\text{-}4)$$

$$D_T|_i = D_T|_{i+1} - \frac{\partial R}{\partial T}\Big|_i \cdot D_C|_{i+1} - \lambda \frac{\partial R}{\partial T}\Big|_i \cdot D_T|_{i+1} \qquad (2.2\text{-}5)$$

with the boundary conditions

$$D_c|_{N+1} = 1 \qquad \text{and} \qquad D_T|_{N+1} = 0$$

where

$$\frac{\partial R}{\partial c}\Big|_i = - k_1(T_i) - k_2(T_i) \tag{2.2-6}$$

$$\frac{\partial R}{\partial T}\Big|_i = k_1(T_i)(1 - c)\frac{E_1}{T^2} - k_2(T_i)\, c\, E_2/T^2 \tag{2.2-7}$$

$$k_1(T_i) = \frac{D_{aI}}{N} e^{E_1 - E_1/T}$$

$$k_2(T_i) = \frac{D_{aI}}{N} e^{E_{02} - E_2/T}$$

3. The direction of the steepest ascent is

$$D_Q|_i = \frac{\partial c}{\partial Q}\Big|_i \cdot D_c|_i + \frac{\partial T}{\partial Q}\Big|_i \cdot D_T|_i \tag{2.2-8}$$

where

$$\frac{\partial c}{\partial Q}\Big|_i = \frac{- \frac{\partial R}{\partial T}\Big|_i}{1 - \frac{\partial R}{\partial c}\Big|_i - \lambda \cdot \frac{\partial R}{\partial T}\Big|_i} \tag{2.2-9}$$

$$\frac{\partial T}{\partial Q}\Big|_i = \frac{- \lambda \frac{\partial R}{\partial T}\Big|_i}{1 - \frac{\partial R}{\partial c}\Big|_i - \lambda \frac{\partial R}{\partial T}\Big|_i} \tag{2.2-10}$$

4. Adjust the heat flux by

$$Q_{New}|_i = Q_{Old}|_i + \frac{D_Q|_i}{\left(\sum_{i=0}^{N} D_Q|_i^2\right)^{1/2}} \cdot P \qquad (2.2\text{-}11)$$

where P is a measure of the total change in Q.

5. Go back to step 1, and calculate the output concentration. If it is less than the previous calculation, halve the value of P in step 4. Otherwise continue the process until no significant improvement can be made.

Starting from the set of Q_i, which maintains the temperature through the reactor at T_o, the heat flux, temperature, and concentration profiles resulting from this method are shown in Figures 1, 2 and 3. The dashed curves indicate the profile at the optimal condition.

The disadvantage of this method of solution is illustrated in Figure 4 by comparison of ΔQ and ΔQ^*. ΔQ^* is the difference between the initial heat flux and the optimal one. As can be seen, the ascending direction is not favorable. In order to explain why this method is not applicable, consider the following example.

Consider a multistage process, where the state variables are related by

$$x_i = x_{i-1} + Q_i \qquad (2.2\text{-}12)$$

$$y_i = y_{i-1} + f_i(x_i) \qquad (2.2\text{-}13)$$

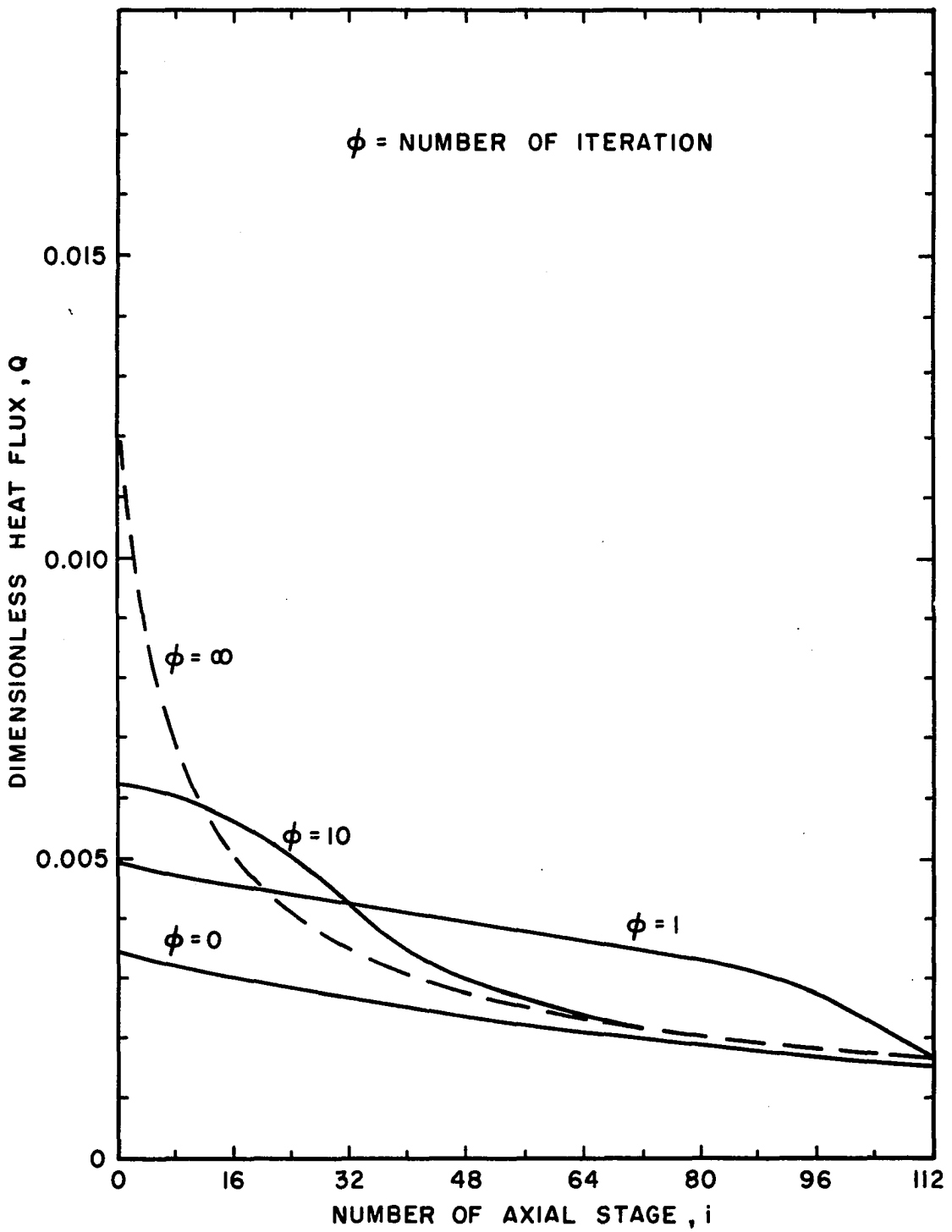


Figure 1.--Dimensionless Heat Flux Profiles of Various Trials and Optimum ($\Phi = \infty$) for One-Dimensional Reactor Model

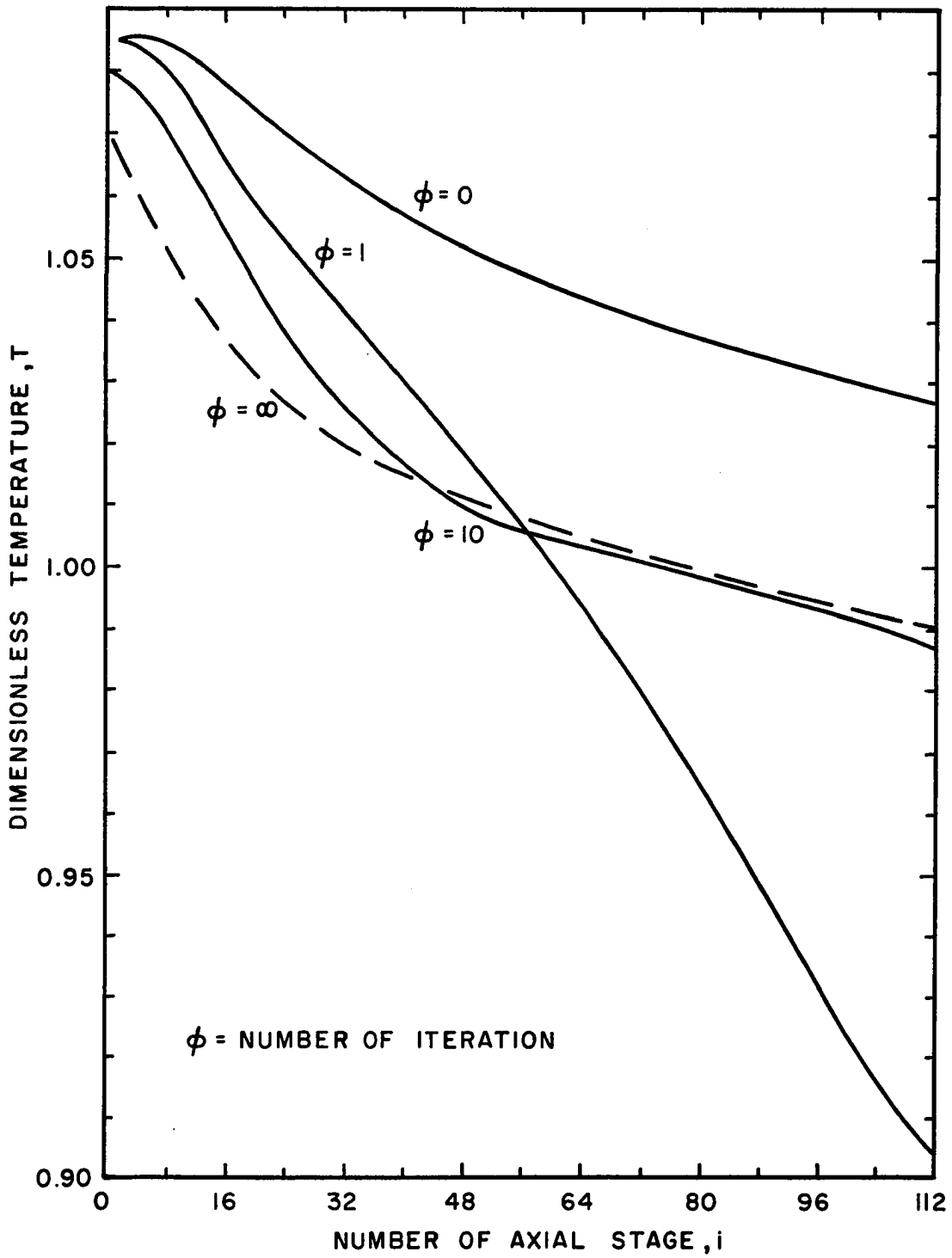


Figure 2.--The Dimensionless Temperature Profiles of Various Trials and Optimum ($\Phi = \infty$) for One-Dimensional Model

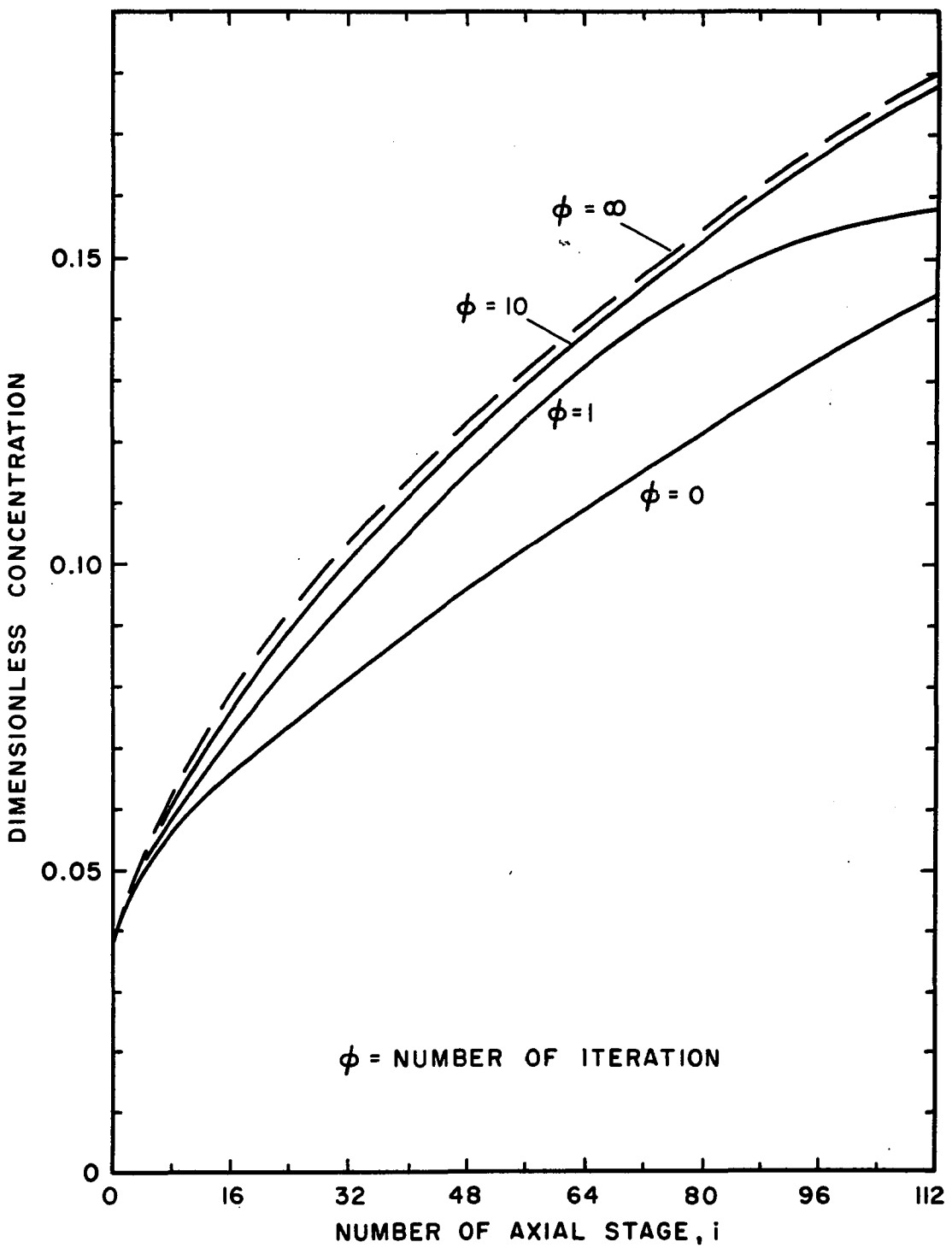


Figure 3.--The Dimensionless Concentration Profiles of Various Trials and Optimum ($\Phi = \infty$) for One-Dimensional Model

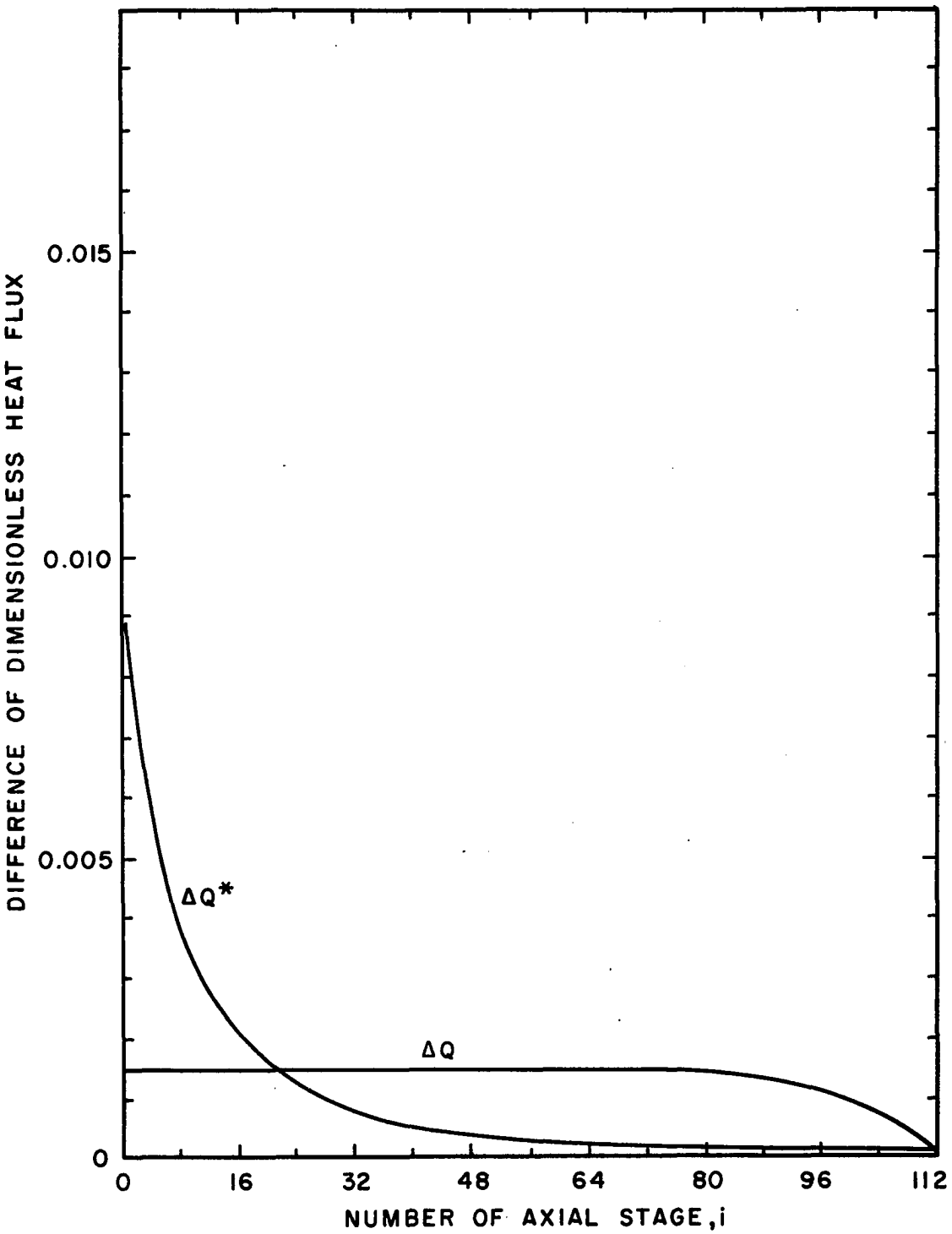


Figure 4.--Comparison of Dimensionless Heat Flux Difference Between the Initial Estimation and the Optimal One (ΔQ^*) and Dimensionless Heat Flux Adjusted in the First Trial (ΔQ)

The initial conditions are

$$x_0 = y_0 = 0 \tag{2.2-14}$$

The term $f_i(x_i)$ is a function of state x_i and location i. Let this function be defined by

$$f_i(x_i) = 10 - (x_i - i)^2 \tag{2.2-15}$$

The objective of this problem is to find a set of control variables, Q_i, which maximize the output, y_N. The solution of this problem can easily be obtained by setting

$$x_i = 1 \qquad \text{for } i = 1, \ldots, N \tag{2.2-16}$$

which corresponds to a set of control variables

$$Q_i = 1 \qquad \text{for } i = 1, \ldots, N \tag{2.2-17}$$

The maximum objective function will be 10 x N.

In order to evaluate the search method we will start at $Q_i = 0$ for $i = 1, \ldots, N$ and then approach the optimal solution by the same technique used before. In this problem, the state variables are x and y. The state adjoint elements can be calculated by

$$D_y|_{i-1} = D_y|_i \tag{2.2-18}$$

$$D_x|_{i-1} = D_x|_i + \frac{\partial f_i}{\partial x_i} \tag{2.2-19}$$

with boundary conditions

$$D_y|_N = 1 \text{ and } D_x|_N = 0 \tag{2.2-20}$$

$$D_y|_i = 1 \quad \text{for } i = 1, \ldots, N \tag{2.2-21}$$

$$D_x|_i = \sum_{j=i}^{N} \frac{\partial f_i}{\partial x_j} = \sum_{j=i}^{N} 2(x_j - j) \quad \text{for } i = 1, \ldots, N \tag{2.2-22}$$

The steepest ascent direction should be

$$D_Q|_i = \frac{\partial x_i}{\partial Q_i} D_x|_i + \frac{\partial y_i}{\partial Q_i} D_y|_i \tag{2.2-23}$$

$$= D_x|_i = 2 \sum_{j=i}^{N} (x_j - j), \text{ for } i = 1, \ldots, N$$

So that the control function is adjusted by

$$Q_{New}|_i = Q_{Old}|_i + D_Q|_i \cdot P \tag{2.2-24}$$

Figure 5 shows the Q curves for the first, second and tenth trials. Figure 6 gives the values of the objective function for the first ten trials. Even though the final yield is quite close to the maximum, the Q curve fails to match the optimal condition. This behavior can be explained as follows:

Since $y_N = Y(Q_1, Q_2, \ldots, Q_N)$, we have

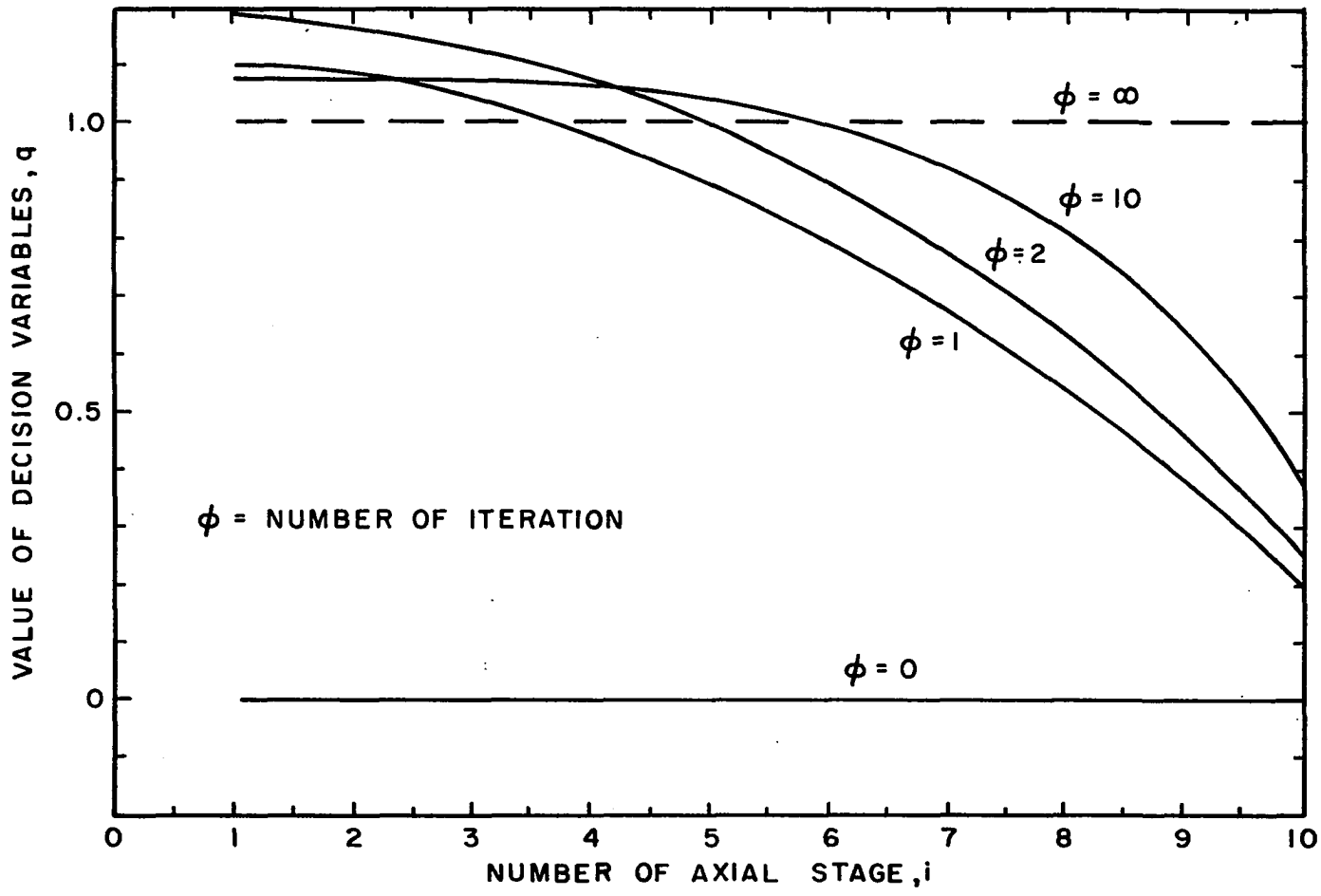


Figure 5.--The Profiles of Decision Variables, q, of Various Trials and Optimal Condition ($\Phi = \infty$)

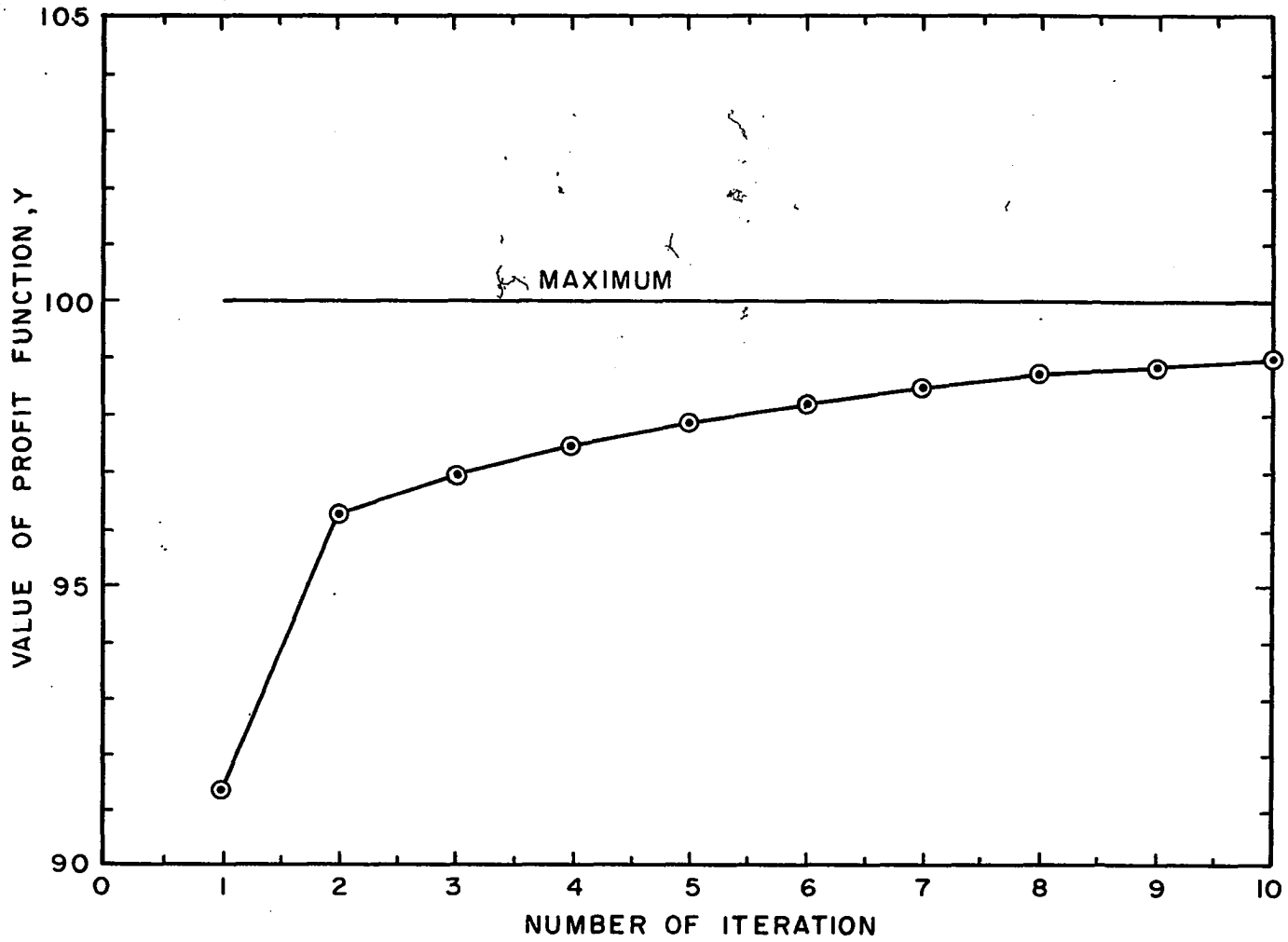


Figure 6.--The Values of Profit Function of Consecutive Trials

$$dY = \frac{\partial Y}{\partial Q_1} dQ_1 + \ldots + \frac{\partial Y}{\partial Q_N} dQ_N \qquad (2.2\text{-}25)$$

Assume that the ΔQ_i's are sufficiently small, so that

$$\Delta Y \simeq \frac{\partial Y}{\partial Q_1} \Delta Q_1 + \ldots + \frac{\partial Y}{\partial Q_N} \Delta Q_N \qquad (2.2\text{-}26)$$

The steepest ascent will be achieved by changing the control variables according to

$$\Delta Q_i = \frac{\partial Y}{\partial Q_i} P \quad \text{for } i = 1, \ldots, N \qquad (2.2\text{-}27)$$

where P is a constant. For this example let

$$P = \frac{\Delta\varphi}{\sum_{i=1}^{N} \left(\frac{\partial Y}{\partial Q_i}\right)^2} \qquad (2.2\text{-}28)$$

So that

$$\Delta Y \simeq \sum_{i=1}^{N} \left[\frac{\partial Y}{\partial Q_i} \cdot \frac{\partial Y}{\partial Q_i} \cdot \frac{\Delta\varphi}{\sum_{j=1}^{N} \left(\frac{\partial Y}{\partial Q_j}\right)^2}\right] = \Delta\varphi \qquad (2.2\text{-}29)$$

However, the first trial for N = 10, $\Delta\varphi$= 559.68 gives ΔY = 376.36, an error of 46%. Incorrect approximation can cause the change of ΔQ_i's away from the steepest ascent. Even though this method is inadequate, it is possible to modify it.

If ΔY is expanded in Taylor's series, we have

$$\Delta Y = \sum_{i=1}^{N} \frac{\partial Y}{\partial Q_i} \Delta Q_i + \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{1}{2!} \frac{\partial^2 Y}{\partial Q_i \partial Q_j} \Delta Q_i \Delta Q_j$$

$$+ \sum_{i} \sum_{j} \sum_{k} \frac{1}{3!} \frac{\partial^3 Y}{\partial Q_i \partial Q_j \partial Q_k} \Delta Q_i \Delta Q_j \Delta Q_k + \ldots \tag{2.2-30}$$

In this example, the second derivative is

$$D_{Q_i Q_j} = \frac{\partial}{\partial Q_i} D_{Q_j} = \frac{\partial}{\partial Q_i} \left[2 \sum_{k=j}^{N} (x_k - k) \right] \tag{2.2-31}$$

Replace x_k by

$$x_k = x_o + \sum_{j=1}^{k} Q_j \tag{2.2-32}$$

then

$$D_{Q_i Q_j} = \frac{\partial}{\partial Q_i} \left[2(x_o + \sum_{k=1}^{j} Q_k - j) + \ldots + 2(x_o + \sum_{k=1}^{N} Q_k - N) \right]$$

$$= \begin{cases} 2(N + 1 - i) & \text{for } j \leq i \leq N \\ 2(N + 1 - j) & \text{for } i < j \leq N \end{cases} \tag{2.2-34}$$

The third and higher derivatives are zero, because the second derivatives are independent of Q_i. To expand the first derivatives by Taylor's series, we have

$$D_{Q_i}(Q_1 + \Delta Q_1, \ldots, Q_N + \Delta Q_N)$$

$$= D_{Q_i}(Q_1, \ldots, Q_N) + \sum_{j=1}^{N} \Delta Q_j \, D_{Q_i Q_j}(Q_1, \ldots, Q_N)$$

$$+ \ldots, \qquad \text{for } i = 1, \ldots, N. \tag{2.2-35}$$

Since the third and higher derivatives are zero, the higher order terms vanish. To attain the maximum directly, the best choice of ΔQ_i's will be those which satisfy

$$D_{Q_i}(Q_1 + \Delta Q_1, \ldots, Q_N + \Delta Q_N) = 0, \text{ for } i = 1, \ldots, N \tag{2.2-36}$$

This is equivalent to solving for the ΔQ_i's from the simultaneous equations

$$D_{Q_i} + \sum_{j=1}^{N} D_{Q_i Q_j} \Delta Q_j = 0 \quad \text{for } i = 1, \ldots, N \tag{2.2-37}$$

The solution in matrix form is

$$\Delta \bar{Q} = - \bar{\bar{D}}_{QQ}^{-1} \bar{D}_Q \tag{2.2-38}$$

where a single bar means a column matrix and a double bar denotes a matrix. The superscript (-1) means the inverse of a matrix. By this procedure, the adjusted Q will exactly attain the optimal conditon. This ascending procedure is called Newton's method [W.2].

In another modification--taking x_i's as the manipulating variables instead of the Q_i's--the interaction between

control variables is also avoidable. In this case, the y_i's are the only state variables. As derived before, the adjoint element

$$D_y|_i = 1, \text{ for } i = 1, \ldots, N \tag{2.2-39}$$

and the steepest ascent direction is

$$D_x|_i = D_y|_i \frac{\partial y_i}{\partial x_i} = 2(x_i - i), \text{ for } i = 1, \ldots, N \tag{2.2-40}$$

This equation is the correct direction leading to the maximum. Here the optimal condition can be found in a single trial, if the proper step size is chosen. This example illustrates the importance of choosing a set of control variables in applying the steepest ascent method.

3. Newton's Method

Returning to the one-dimensional reactor problem, first directly apply Newton's method. The second order derivatives are

$$\frac{\partial}{\partial Q_j} D_Q|_i = \frac{\partial}{\partial Q_j}\left[\frac{\partial c_i}{\partial Q_i} D_c|_i + \frac{\partial T_i}{\partial Q_i} D_T|_i\right] \tag{2.3-1}$$

For $i \le j \le N$, $\frac{\partial c_i}{\partial Q_i}$ and $\frac{\partial T_i}{\partial Q_i}$ are independent of Q_i, leading to

$$\frac{\partial}{\partial Q_j} D_Q|_i = \frac{\partial c_i}{\partial Q_i}\frac{\partial c_j}{\partial Q_j}\frac{\partial}{\partial c_j} D_c|_i + \frac{\partial c_i}{\partial Q_i}\frac{\partial T_j}{\partial Q_j}\frac{\partial}{\partial T_j} D_c|_j$$

$$+ \frac{\partial T_i}{\partial Q_i} \frac{\partial c_j}{\partial Q_j} \frac{\partial}{\partial c_j} D_T|_i + \frac{\partial T_i}{\partial Q_i} \frac{\partial T_j}{\partial Q_j} \frac{\partial}{\partial T_j} D_T|_i \qquad (2.3\text{-}2)$$

Denote the second order state adjoint elements by

$$\frac{\partial}{\partial c_j} D_c|_i = D_{cc}|_{i,j}$$

$$\frac{\partial}{\partial T_j} D_c|_i = D_{cT}|_{i,j}$$

$$\frac{\partial}{\partial c_j} D_T|_i = D_{Tc}|_{i,j}$$

$$\frac{\partial}{\partial T_j} D_T|_i = D_{TT}|_{i,j}$$

Replace the first order adjoints by equations (2.2-4) and (2.2-5), then

$$\frac{\partial}{\partial c_j} D_c|_i = \frac{\partial}{\partial c_j} \left[D_c|_{i+1} - \frac{\partial R}{\partial c}|_i \, D_c|_{i+1} - \lambda \frac{\partial R}{\partial c}|_i \, D_T|_{i+1} \right] \qquad (2.3\text{-}3)$$

If $i < j$, $\frac{\partial R}{\partial c}|_i$ is independent of c_j

$$D_{cc}|_{i,j} = D_{cc}|_{i+1,j} - \frac{\partial R}{\partial c}|_i \, D_{cc}|_{i+1,\,j} - \lambda \frac{\partial R}{\partial c}|_i \, D_{Tc}|_{i+1,j} \qquad (2.3\text{-}4)$$

If $i = j$, then

$$D_{cc}|_{jj} = D_{cc}|_{j+1,j} - \frac{\partial^2 R}{\partial c^2}|_j \; (D_c|_{i+1} + \lambda \, D_T|_{i+1})$$

$$- \frac{\partial R}{\partial c}|_j \; (D_{cc}|_{j+1,j} + \lambda \, D_{Tc}|_{j+1,j}) \qquad (2.3\text{-}5)$$

Boundary conditions are

$$D_c|_{N+1} = 1$$

$$D_T|_{N+1} = D_{cc}|_{N+1,\ N+1} = D_{TT}|_{N+1,\ N+1} = D_{cT}|_{N+1,\ N+1} = 0$$

Other second order adjoints are

$$D_{Tc}|_{i,j} = \frac{\partial}{\partial T_j} \left[D_c|_{i+1} - \frac{\partial R}{\partial c}|_i \, D_c|_{i+1} - \lambda \, \frac{\partial R}{\partial c}|_i \, D_T|_{i+1} \right]$$

$$= D_{Tc}|_{i+1} - \frac{\partial R}{\partial c}|_i \; (D_{cT}|_{i+1,j} + \lambda \, D_{TT}|_{i+1,j})$$

$$- (\bar{\delta}_i \cdot \bar{\delta}_j) \, \frac{\partial^2 R}{\partial c \partial T}|_i \; (D_c|_{i+1} + \lambda \, D_T|_{i+1}) \qquad (2.3\text{-}6)$$

$$D_{cT}|_{i,j} = D_{cT}|_{i+1,j} - \frac{\partial R}{\partial T}|_i \; (D_{cc}|_{i+1,j} + \lambda \, D_{Tc}|_{i+1,j})$$

$$- (\bar{\delta}_i \cdot \bar{\delta}_j) \, \frac{\partial^2 R}{\partial c \partial T}|_i \; (D_c|_{i+1} + \lambda \, D_T|_{i+1}) \qquad (2.3\text{-}7)$$

$$D_{TT}|_{i,j} = D_{TT}|_{i+1,j} - \frac{\partial R}{\partial T}|_i \; (D_{cT}|_{i+1,j} + \lambda \, D_{TT}|_{i+1,j})$$

$$- (\bar{\delta}_i \cdot \bar{\delta}_j) \, \frac{\partial^2 R}{\partial T^2}|_i \; (D_c|_{i+1} + \lambda \, D_T|_{i+1}) \qquad (2.3\text{-}8)$$

where $\bar{\delta}_i$ and $\bar{\delta}_j$ are unit vectors with the following properties

$$(\bar{\delta}_i \cdot \bar{\delta}_j) = 1 \quad \text{for } i = j \tag{2.3-9}$$

$$(\bar{\delta}_i \cdot \bar{\delta}_j) = 0 \quad \text{for } i \neq j \tag{2.3-10}$$

Equations (2.3-5), (2.3-6), (2.3-7) and (2.3-8) were obtained for the conditions $i \leq j \leq N$. However, if $j < i \leq N$, the same relations can be obtained, but the position of i and j is exchanged. The second order derivatives of the reaction rate with respect to temperature and concentration are

$$\frac{\partial^2 R}{\partial T^2} = \frac{k_1 E_1 (1 - c)}{T^3}\left(\frac{E_1}{T} - 2\right) - \frac{k_2 E_2 c}{T^3}\left(\frac{E_2}{T} - 2\right) \tag{2.3-11}$$

$$\frac{\partial^2 R}{\partial c \partial T} = -\frac{k_1 E_1 + k_2 E_2}{T^2} \tag{2.3-12}$$

$$\frac{\partial^2 R}{\partial c^2} = 0 \tag{2.3-13}$$

where

$$k_1 = \frac{D_{aI}}{N} \exp\,(E_1 - E_1/T)$$

$$k_2 = \frac{D_{aI}}{N} \exp\,(E_{02} - E_2/T) \tag{2.3-14}$$

The computational procedure can be summarized as follows:

1. Estimate a reasonable heat flux profile for each of N stages along the reactor, calculate the temperature, concentration and the following terms

$$\frac{\partial R}{\partial c}, \frac{\partial R}{\partial T}, \frac{\partial^2 R}{\partial c \partial T}, \frac{\partial^2 R}{\partial T^2}$$

2. Integrate the first order adjoint as shown in the previous section.

3. Starting at j = N evaluate

$$D_{cc}|_{i,j}, D_{cT}|_{i,j}, D_{Tc}|_{i,j}, \text{ and } D_{TT}|_{i,j}$$

for i from N to 1, by equations (2.3-5), (2.3-6), (2.3-7) and (2.3-8). Then repeat the procedure for all other j.

4. Compute $\frac{\partial c_i}{\partial Q_i}$ and $\frac{\partial T_i}{\partial Q_i}$ by equation (2.2-9) and (2.2-10) for all i.

5. Obtain $D_Q|_i$ by equation (2.2-8).

6. Calculate $\frac{\partial}{\partial Q_j} D_Q|_i$ by equation (2.3-2) for i from 1 to N, and j from 1 to N.

7. Invert the matrix $\bar{\bar{D}}_{QQ}$, of which the (i,j)-th element is $\frac{\partial}{\partial Q_j} D_Q|_i$

8. Multiply the new matrix $\bar{\bar{D}}_{QQ}^{-1}$ by $\bar{D}_Q$, where $\bar{D}_Q$ is a column matrix, its i-th element is $D_Q|_i$

9. Adjust the control function by

$$\bar{Q}_{New} = \bar{Q}_{Old} - \bar{\bar{D}}_{QQ}^{-1} \cdot \bar{D}_Q \qquad (2.3\text{-}15)$$

10. Repeat the procedure from step 1, until all the elements in D_Q are zero, or no significant improvement on the yield can be made.

The computation time and the required memory storage increase by the second power of stage number. For N equal 112 the capacity of the Osage computer [0.1] currently used was exceeded. Therefore, N is taken to be 28, instead of 112. All other constants remain unchanged. Some results for two different initial conditions are given in Table 2 and Table 3.

The following conclusions can be drawn from the results as shown on Tables 2 and 3.

1. The second order derivatives are quite large in comparison with the first derivatives. Therefore, neglecting higher order terms, as is done in the gradient method, can cause serious errors.

2. The amount of variation of the second derivatives indicate that in addition the third and higher order terms cannot be neglected. This points out the possible error in applying Newton's method.

3. We note that in Table 2, the first two columns of $\bar{\bar{D}}_{QQ}$ are very close to each other, which implies that the matrix is ill-conditioned. Therefore we would expect extreme difficulty in obtaining the inverse of $\bar{\bar{D}}_{QQ}$. If this is the case Newton's method is not practical and will in general fail to converge.

TABLE 2

FIRST AND SECOND ORDER ADJOINTS OF HEAT FLUX

i	c_i	T_i	$Q_i \times 100$	$D_Q\|_i$	$\frac{\partial}{\partial Q_j} D_{Q_i}$			
					j = 1	j = 2	j = 14	j = 15
0	0.0382	1.0760						
1	0.0485	1.0834	1.333	0.3834	-0.0483	-0.0484	-0.1287	-0.6000
2	0.0542	1.0789	1.295	0.3834	-0.0484	-0.0484	-0.1288	-0.6000
3	0.0600	1.0770	1.257	0.3834	-0.0484	-0.0485	-0.1288	-0.6000
4	0.0651	1.0744	1.221	0.3834	-0.0486	-0.0487	-0.1290	-0.6000
5	0.0694	1.0716	1.186	0.3834	-0.0490	-0.0491	-0.1294	-0.6001
6	0.0739	1.0685	1.151	0.3834	-0.0497	-0.0498	-0.1302	-0.6002
7	0.0779	1.0653	1.118	0.3833	-0.0510	-0.0511	-0.1317	-0.6005
8	0.0818	1.0623	1.086	0.3833	-0.0533	-0.0533	-0.1344	-0.6009
9	0.0856	1.0593	1.054	0.3832	-0.0570	-0.0571	-0.1394	-0.6018
10	0.0893	1.0564	1.024	0.3831	-0.0628	-0.0629	-0.1479	-0.6032
11	0.0930	1.0537	0.994	0.3829	-0.0717	-0.0717	-0.1619	-0.6056
12	0.0965	1.0512	0.966	0.3826	-0.0846	-0.0847	-0.1845	-0.6095
13	0.1000	1.0488	0.938	0.3821	-0.1032	-0.1032	-0.2201	-0.6155
14	0.1035	1.0466	0.911	0.3813	-0.1287	-0.1287	-0.2745	-0.6248
15	0.1068	1.0444	0.884	0.3801	-0.1632	-0.1632	-0.3041	-0.6387
16	0.1101	1.0424	0.859	0.3783	-0.2082	-0.2082	-0.3442	-0.6590
17	0.1134	1.0405	0.834	0.3758	-0.2656	-0.2656	-0.3967	-0.6886
18	0.1165	1.0387	0.810	0.3722	-0.3371	-0.3371	-0.4632	-0.7308
19	0.1196	1.0371	0.786	0.3672	-0.4234	-0.4234	-0.5442	-0.7903
20	0.1226	1.0354	0.764	0.3601	-0.5242	-0.5242	-0.6394	-0.8730
21	0.1256	1.0339	0.742	0.3505	-0.4375	-0.4375	-0.7464	-0.9867
22	0.1285	1.0325	0.720	0.3373	-0.7582	-0.7582	-0.8603	-1.1415
23	0.1313	1.0312	0.700	0.3195	-0.8777	-0.8777	-0.9719	-1.3506
24	0.1340	1.0299	0.679	0.2957	-0.9814	-0.9814	-1.0663	-1.6308
25	0.1367	1.0287	0.660	0.2639	-1.0469	-1.0469	-1.1209	-2.0036
26	0.1394	1.0275	0.641	0.2220	-1.0408	-1.0408	-1.1016	-2.4968
27	0.1420	1.0265	0.622	0.1667	-0.9148	-0.9148	-0.9595	-3.1459
28	0.1444	1.0255	0.604	0.0944	-0.5999	-0.5999	-0.6248	-3.9962

TABLE 3

FIRST AND SECOND ORDER ADJOINTS OF HEAT FLUX
AT UNIFORM TEMPERATURE DISTRIBUTION

i	c_i	T_i	$Q_i \times 100$	$D_Q\|_i$	$\frac{\partial}{\partial Q_j} D_Q\|_i$			
					j = 1	j = 2	j = 14	j = 28
0	0.0382	1.076						
1	0.0447	1.00	8.932	-1.6981	-1520.6	-1241.3	-236.0	-212.8
2	0.0512	1.00	1.294	-1.3236	-1241.3	-1010.3	-193.1	-174.2
3	0.0576	1.00	1.256	-1.0379	-1027.5	-836.7	-160.4	-144.8
4	0.0637	1.00	1.220	-0.8169	-861.4	-701.7	-135.1	-122.0
5	0.0697	1.00	1.185	-0.6438	-730.6	-595.4	-115.3	-104.2
6	0.0755	1.00	1.151	-0.5066	-626.1	-510.4	-99.5	-90.0
7	0.0811	1.00	1.117	-0.3967	-541.7	-441.8	-87.0	-78.7
8	0.0866	1.00	1.085	-0.3079	-472.6	-385.6	-76.8	-69.5
9	0.0919	1.00	1.054	-0.2353	-415.4	-339.1	-68.5	-62.1
10	0.0971	1.00	1.023	-0.1758	-367.5	-300.1	-61.6	-55.9
11	0.1021	1.00	0.994	-0.1265	-327.0	-267.1	-56.0	-50.8
12	0.1070	1.00	0.965	-0.0857	-292.3	-238.9	-51.3	-46.6
13	0.1117	1.00	0.937	-0.0517	-262.3	-214.5	-47.4	-43.1
14	0.1163	1.00	0.910	-0.0234	-236.0	-193.1	-44.2	-40.2
15	0.1207	1.00	0.884	-0.0000	-212.8	-174.2	-40.2	-37.8
16	0.1250	1.00	0.858	0.0192	-192.1	-157.3	-36.6	-34.5
17	0.1292	1.00	0.834	0.0349	-173.4	-142.0	-33.4	-31.4
18	0.1333	1.00	0.810	0.0473	-156.2	-128.1	-30.4	-28.6
19	0.1372	1.00	0.786	0.0567	-140.3	-115.1	-27.5	-26.0
20	0.1410	1.00	0.764	0.0634	-125.4	-102.9	-24.9	-23.4
21	0.1447	1.00	0.741	0.0674	-111.2	-91.3	-22.2	-21.0
22	0.1483	1.00	0.720	0.0689	-97.6	-80.2	-19.7	-18.6
23	0.1518	1.00	0.699	0.0678	-84.2	-69.2	-17.2	-16.3
24	0.1551	1.00	0.679	0.0641	-71.0	-58.4	-14.6	-13.9
25	0.1584	1.00	0.660	0.0577	-57.7	-47.5	-12.0	-11.4
26	0.1616	1.00	0.640	0.0483	-44.2	-36.4	-9.3	-8.8
27	0.1647	1.00	0.622	0.0358	-30.2	-24.9	-6.4	-6.1
28	0.1677	1.00	0.604	0.0198	-15.5	-12.8	-3.3	-3.2

4. Other Methods

If the stage temperatures are chosen as the manipulative variable, the concentration becomes the only state variable. The adjoint of the state variable can be evaluated as follows:

$$D_c|_i = D_c|_{i+1} - \frac{\partial R}{\partial c}\Big|_i D_c|_{i+1} \qquad (2.4\text{-}1)$$

with the boundary condition

$$D_c|_{N+1} = 1 \qquad (2.4\text{-}2)$$

The gradient direction is

$$D_T|_i = \frac{\partial c_i}{\partial T_i} D_c|_i = \frac{\partial R_i}{\partial T_i} D_c|_i \qquad \text{for } i = 1, \ldots, N \qquad (2.4\text{-}3)$$

The computation procedure is similar to that of section 2.

Figure 7 shows the temperature distributions for three consecutive trials and the optimal condition. We see that the successive approximations are in the right direction and hence can expect the method to converge. However, Figure 7 indicates the convergence to be slow. Therefore we must explore other methods which will give faster convergence to the desired optimum.

In the first section of this chapter, we derived the disjoint property of a reversible reaction. It states that in a one-dimensional tubular reactor, the optimal

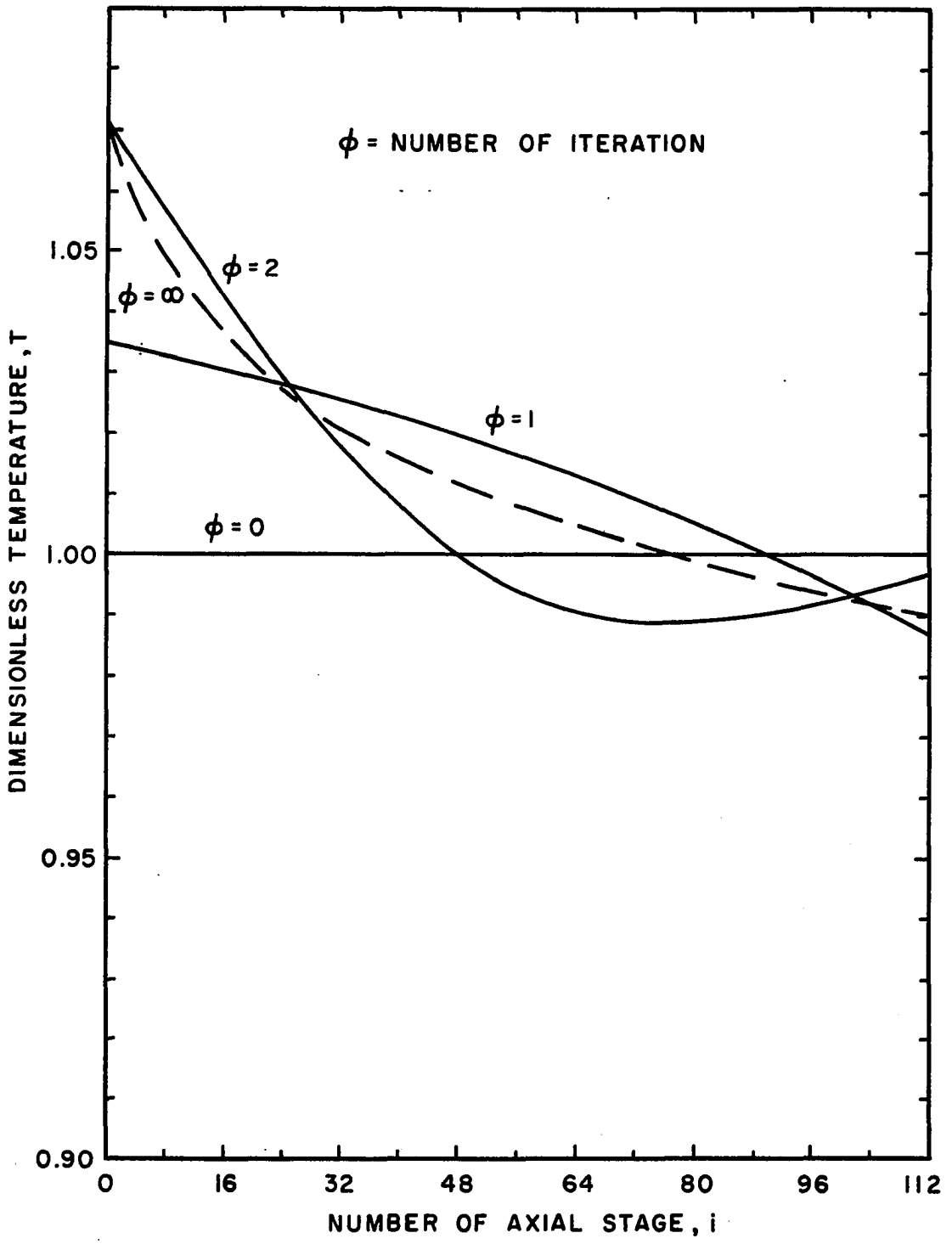


Figure 7.--Dimensionless Temperature Profiles of Consecutive Trials and Optimal Condition for One-Dimensional Reactor Model

temperature for a reversible reaction is a function of local concentration only, regardless of the length of reactor or the other decisions.

In equation (2.4-3), $\frac{\partial R_i}{\partial T_i}$ is a function of local concentration only, but the factor $D_c|_i$ will depend on the state function of other stages as well. It indicates that including the factor $D_c|_i$ in the ascending direction might not be advisable. In addition, if we succeed in attaining a state trajectory at which

$$\frac{\partial R}{\partial T}\Big|_i = 0 \qquad \text{for } i = 1, 2, \ldots, N \tag{2.4-4}$$

then

$$\frac{\partial c_{N-1}}{\partial T_i} = \frac{\partial c_{N-1}}{\partial c_N}\Big|_{T_N} \cdot \frac{\partial c_N}{\partial c_{N-1}}\Big|_{T_{N-1}} \cdots \frac{\partial c_i}{\partial T_i} = 0 \tag{2.4-5}$$

Therefore, it satisfies the necessary condition for the existence of an optimum.

Figure 8 shows the result of three consecutive trials based on

$$\Delta Q_i = \frac{\partial R}{\partial T}\Big|_i \cdot P , \qquad \text{for } i = 1, \ldots, N \tag{2.4-6}$$

The third trial is almost identical with the optimal profile. So far, this procedure is the most successful search technique for this problem. We shall further test its reliability by starting from different initial conditions.

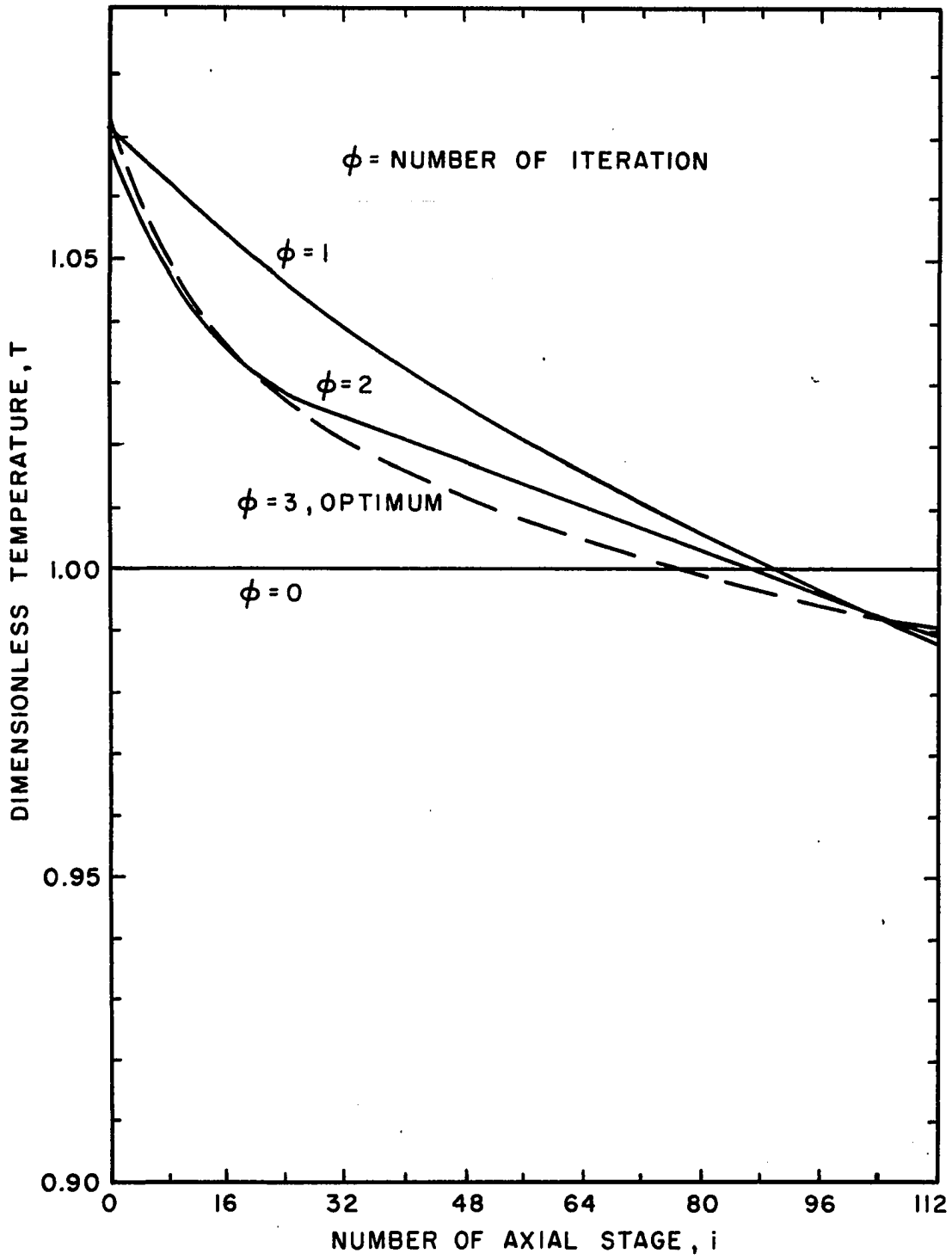


Figure 8.--Dimensionless Temperature Profiles of Consecutive Trial for One-Dimensional Reactor Model

Figure 9 shows the convergence to the optimal profile when started from an extremely bad estimation of the initial conditions. This figure shows that the method will not converge for all initial conditions. The reason for this failure is that $\frac{\partial R}{\partial T}$ does not increase monotonically with decreasing temperature. Figure 10 gives the reaction rate versus temperature with concentration as a parameter. Although the curves are unimodal, the gradient becomes flat as the temperature decreases. Figure 11 indicates this phenomenon more clearly. Around the optimal point the curves of $\frac{\partial R}{\partial T}$ versus T are almost straight lines with negative slope. As T decreases we see that the slope of $\frac{\partial R}{\partial T}$ changes signs. Therefore, it is suggested that the direction of ascent, $\frac{\partial R}{\partial T}$, should be linearized to avoid this problem.

The linearization can be carried out as below

$$D_Q|_i = a\ T_i + b \qquad (2.4\text{-}7)$$

where both a and b are functions of concentration only. At the optimal temperature, T_i^*

$$D_Q|_i = 0 \qquad (2.4\text{-}8)$$

and

$$a\ T_i^* + b = 0 \qquad (2.4\text{-}9)$$

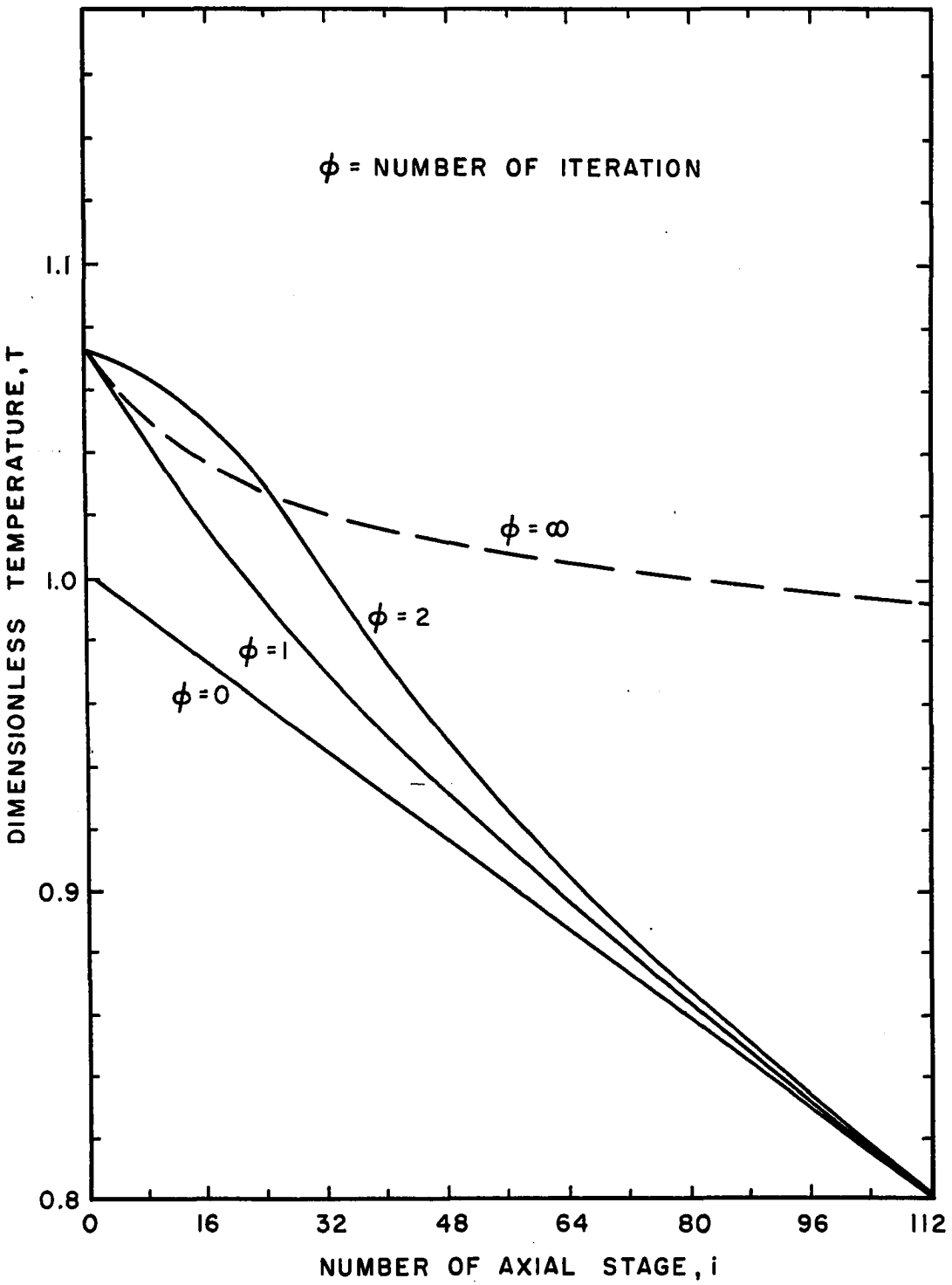


Figure 9.--Dimensionless Temperature Profiles of Consecutive Trials and Optimal Condition ($\Phi = \infty$) for One-Dimensional Reactor Model

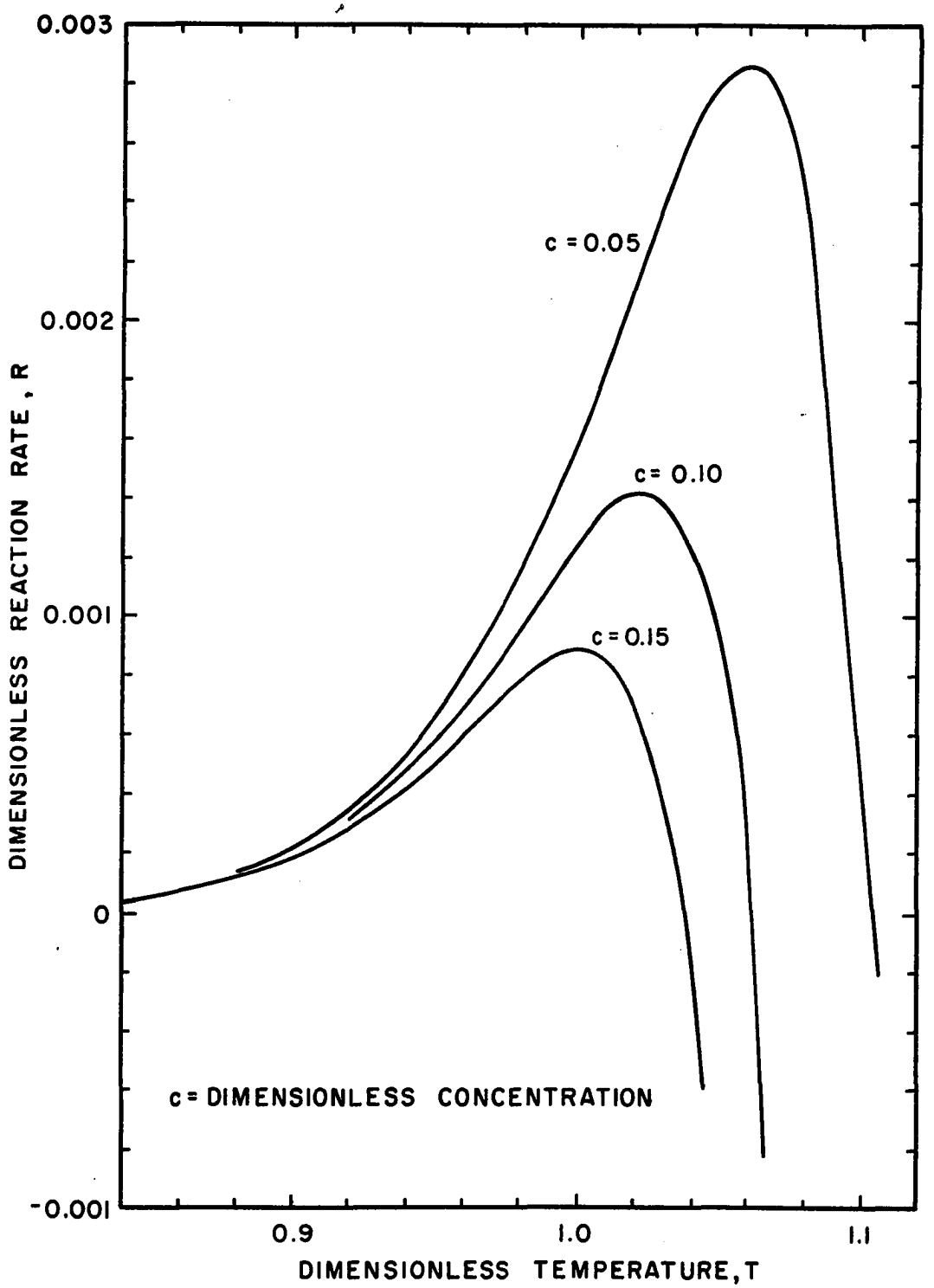


Figure 10.--Reactor Rate Versus Temperature at Various Concentration

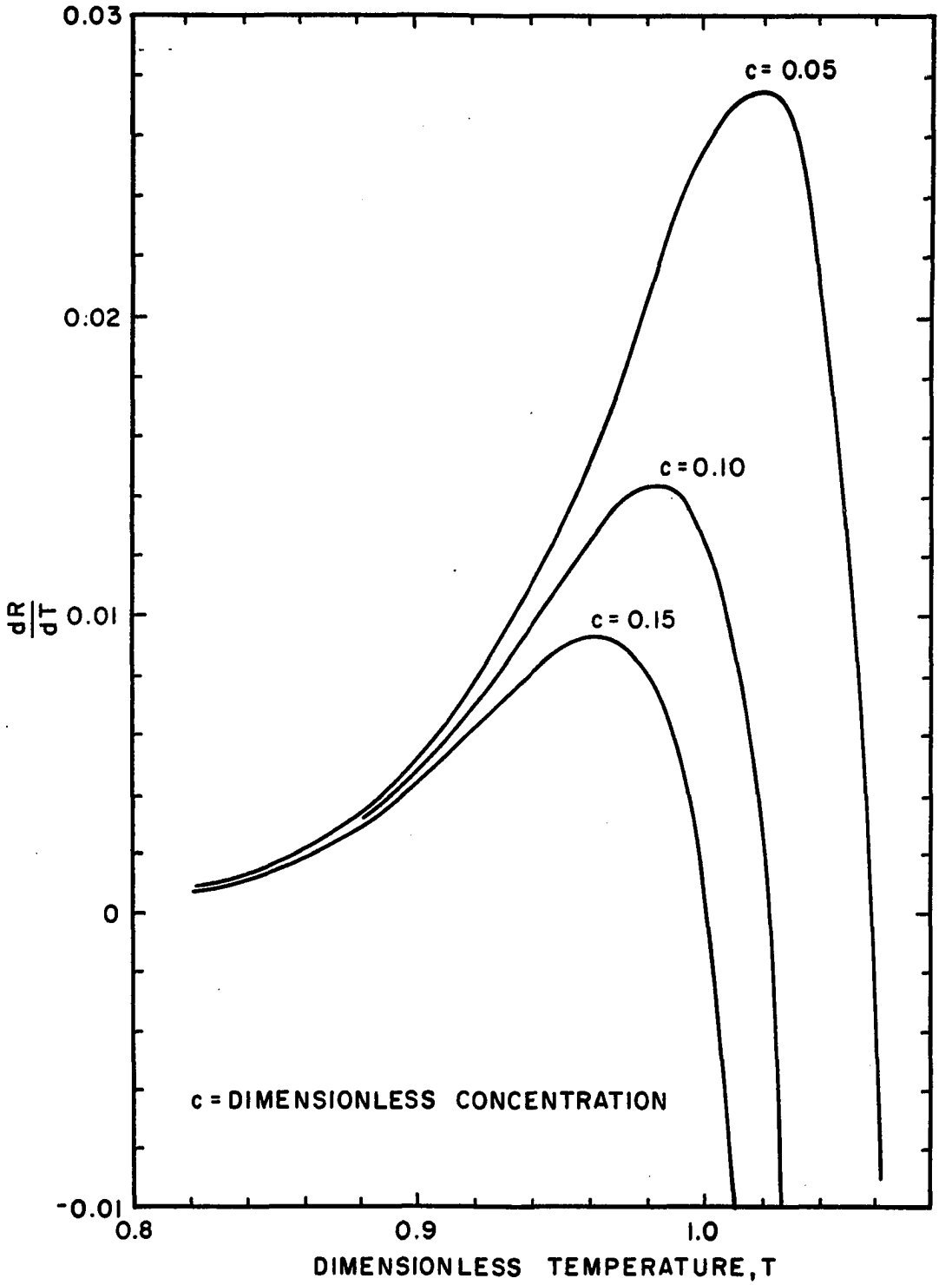


Figure 11.-- $\frac{\partial R}{\partial T}$ versus T at Various Concentrations

Solving (2.4-9) for b and substituting it into the original equation results in

$$D_Q|_i = a\ (T_i - T_i^*) \qquad (2.4\text{-}10)$$

However, our goal is to attain a trajectory at which

$$T_i = T_i^* \qquad \text{for } i = 1, \ldots, N \qquad (2.4\text{-}11)$$

So the factor a can be chosen to be unity or a proportional constant, P.

$$D_Q|_i = P\ (T_i - T_i^*) \qquad (2.4\text{-}12)$$

Starting at the isothermal temperature of unity, the results of two temperature profiles by this ascending direction are given in Figure 12. Figure 13 gives the results starting from a bad initial guess. In both cases the second trials match with the optimal condition. Therefore, the convergence of this method of solution apparently does not depend on the choice of the initial conditions.

5. Conclusion

The optimal policy for the reversible reaction in a single dimensional tubular reactor has been established analytically. The result was used as a basis of comparison for finding a suitable search technique which can be applied to more complicated problems.

The comprehensive study of search techniques was summarized in five methods. The first method, which is

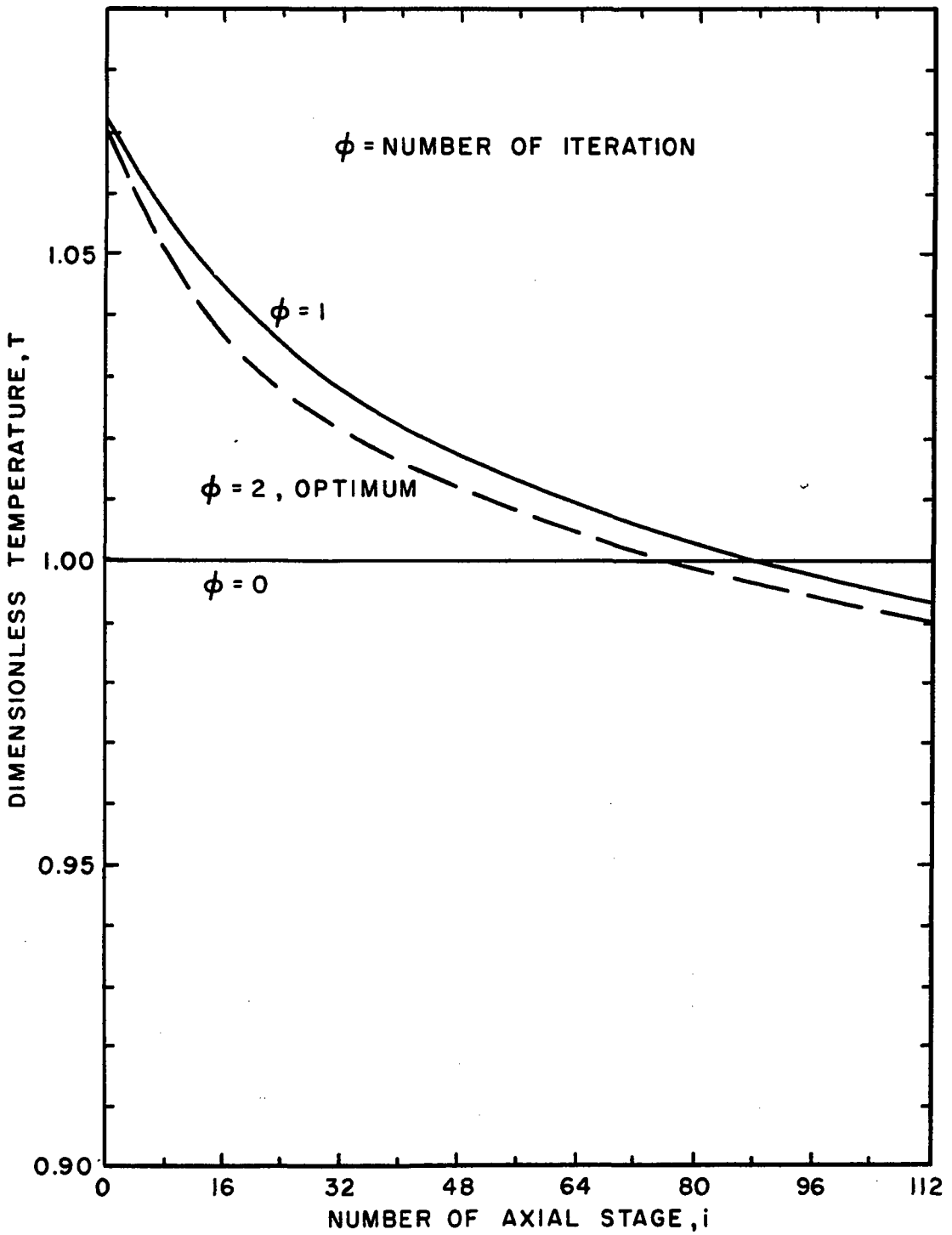


Figure 12.--Dimensionless Temperature Profiles of Consecutive Trials for One-Dimensional Reactor Model

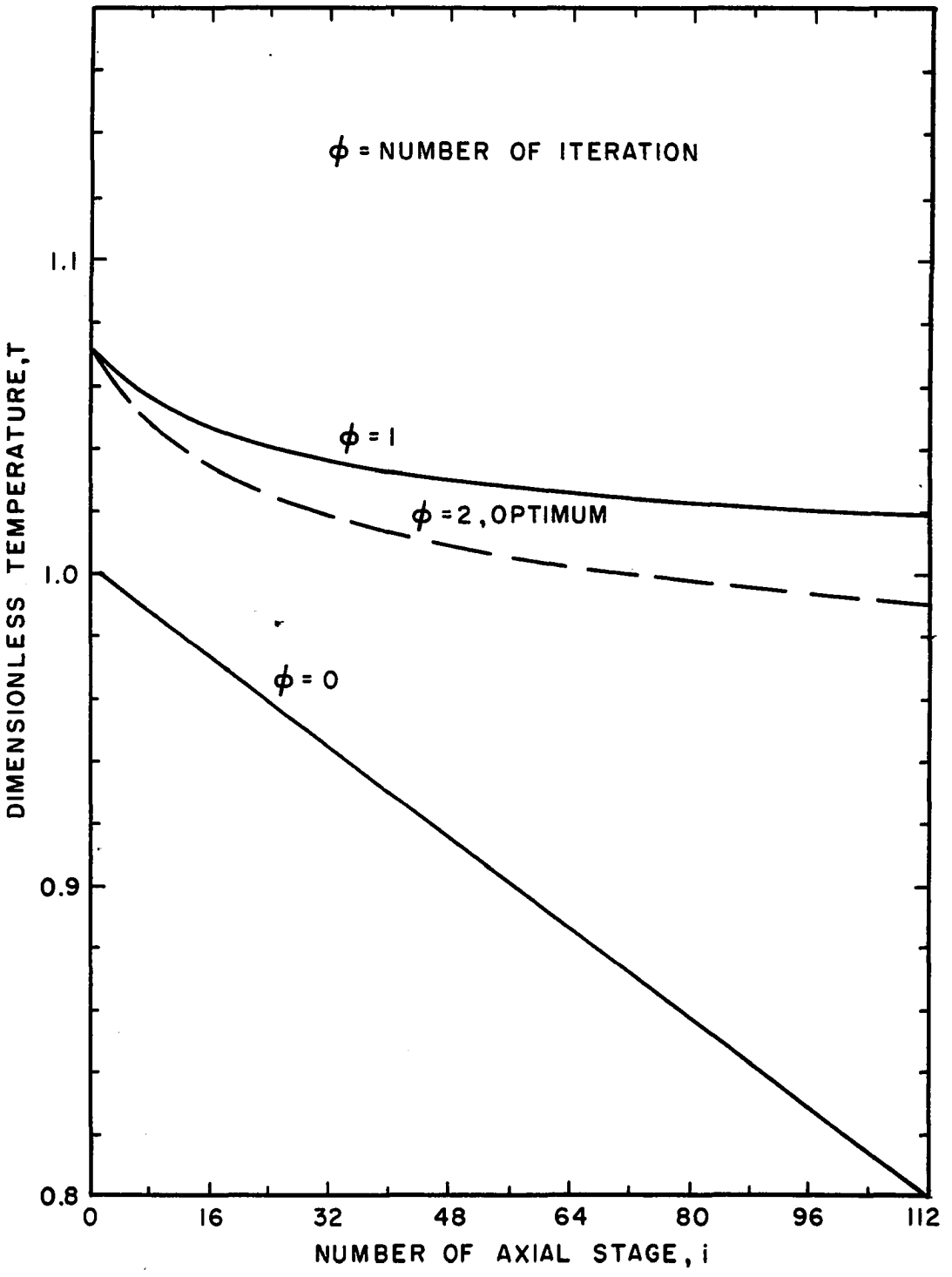


Figure 13.--Dimensionless Temperature Profiles of Consecutive Trials for One-Dimensional Reactor Model

similar to the method used by Gray for an optimal heat flux search of a two-dimensional reactor, was found inadequate because of the interaction between control variables. In the second method, an attempt was made to correct the interaction problem by including the second order terms. This was not applicable either due to the error in neglecting the third and higher order derivatives. By choosing the stage temperatures as the manipulative variables, the results of the third method is improved but is not yet satisfactory. Adopting the concept of the disjoint property of a reversible reaction, the local rate gradient was used in the next method as the ascending direction. The method worked satisfactorily for some initial conditions, but it failed for others.

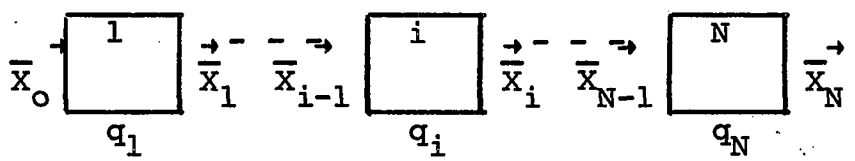
Further improvement by changing the stage temperature to the optimal temperature value based on the local concentration was made in the last approach, then this method worked successfully for all calculated cases.

CHAPTER III

PSEUDO-OPTIMUM SEARCH METHOD

1. Development of the Method

Consider a multistage decision process, illustrated in the diagram



The objective function is

$$Y = Y(\bar{X}_N)$$

The transformation functions are

$$\bar{X}_i = \bar{F}_i(\bar{X}_{i-1}; q_i), \text{ for } i = 1, \ldots, N \qquad (1.3\text{-}1)$$

where X_i is a column matrix with $x_i^1, x_i^2, \ldots, x_i^S$ as its entries. Introduce the Hamiltonian function

$$H_i = \sum_{s=1}^{S} z_i^s F_i^s, \qquad (1.3\text{-}2)$$

$$z_i^s = \frac{\partial H_i}{\partial x_{i-1}^s}, \qquad (1.3\text{-}3)$$

for $s = 1, \ldots, S$ and $i = 1, \ldots, N$

The maximum principle gives the necessary condition of optimum as

$$\frac{\partial H_i}{\partial q_i} = 0, \text{ for } i = 1, \ldots, N \qquad (1.3\text{-}11)$$

or

$$H_i = \text{Maximum, for } i = 1, \ldots, N \qquad (1.3\text{-}12)$$

It is assumed that the initial condition $\bar{X}_0$ is fixed, then the decisions $q_1 \ldots, q_N$ are the only independent variables. A perturbation of Y can be expressed as

$$\delta Y = \frac{\partial Y}{\partial q_1} \delta q_1 + \ldots + \frac{\partial Y}{\partial q_N} \delta q_N \qquad (3.1\text{-}1)$$

and Equation (1.3-10) also gives

$$\delta Y = \frac{\partial H_1}{\partial q_1} \delta q_1 + \ldots \frac{\partial H_N}{\partial q_N} \delta q_N$$

Since the disturbances δq_1 to δq_N are small but arbitrary, we might choose all of them to be zero but δq_i. Then Equation (3.1-1) gives

$$\delta Y = \frac{\partial Y}{\partial q_i} \delta q_i \qquad (3.1\text{-}2)$$

while Equation (1.3-10) gives

$$\delta Y = \frac{\partial H_i}{\partial q_i} \delta q_i \qquad (3.1\text{-}3)$$

Therefore, we have

$$\frac{dY}{dq_i} = \frac{dH_i}{dq_i} \qquad (3.1\text{-}4)$$

where i can be any integer between 1 and N. Integrating (3.1-4) with respect to q_i, we obtain

$$Y = H_i + \text{constant}, \qquad (3.1\text{-}5)$$

where all decisions except q_i remain constant. Then from equation (1.3-12) it can be induced that

$$q_i : \text{Max } Y(q_i)|q_{j\neq i}, \text{ for } i = 1, \ldots, N \qquad (3.1\text{-}6)$$

This notation means q_i is chosen to maximize the objective function, Y, while all decisions other than q_i remain constant. In general the solution of equation (1.3-11) or equation (3.1-6) is very difficult or even impossible to carry out. However, it is quite practical to obtain a solution for a single equation as

$$q_1 : \text{Max } Y(q_1)|q_{j\neq 1} \qquad (3.1\text{-}7)$$

Define the solution of the above equation to be q_1^*. Similarly, we find all other q_i^*. Therefore, we have a N-dimensional vector $\bar{Q}^*$. In general, q_i^* is a function of the other variables, for example:

$$q_1^* = f(q_2, q_3, \ldots, q_N) \qquad (3.1\text{-}8)$$

Let $\bar{Q}^*$ be called the pseudo-optimum. If $\bar{Q}^*$ is independent of $\bar{Q}$, then it will be the optimum. However, since q_i^* is, in general, a function of the other variables, the calculated $\bar{Q}^*$ will not be the optimal one. The author suggests that $\bar{Q}^*$ might still provide a good estimation for next trial. The last method of solution used in the one-dimensional reactor problem uses this technique which was proved to provide better convergence than any of the other used search methods.

The general computational procedure is given as follows:

1. Estimate starting values of $q_1, q_2, \ldots, q_N$.

2. Based on the values of $q_2, \ldots, q_N$ calculate a value for q_1 which gives the largest Y. Denote it as q_1^*.
3. Similarly, calculate q_2^* based on $q_1, q_3, \ldots, q_N$ and so on for the rest of q_1^*.
4. Replace q_i by q_i^* for all of N decisions. Then repeat the cycle from step 2, until the calculated $\bar{Q}^*$ matches with the estimated $\bar{Q}$, or the difference between each of their components is smaller than a tolerable error.

A modification of this method is to make an ascent in the direction leading toward $\bar{Q}^*$, but not necessarily reaching the point $(q_i^*, \ldots, q_N^*)$. Written in mathematical form, this can be stated as

$$q_i|_{new} = q_i|_{old} + \Delta(q_i^* - q_i|_{old}) \text{ for } i = 1, 2, \ldots, N \quad (3.1\text{-}9)$$

where Δ is a number between zero and unity. Since Δ is a variable, the best value of Δ will be that for which the yield, resulting from decisions described by Equation (3.1-9), is the maximum. For most problems, it is difficult (even impossible) to obtain an analytical solution for the optimal Δ. However, it is possible to use a one-dimensional search technique to find the best Δ. In general, the one-dimensional search methods are elegant and powerful. For example, the Golden Section method can locate the maximum within an interval less than one percent of the original estimated range after eleven trials. For more information concerning these methods, Wilde's book Optimum Seeking Methods [W.1] is recommended.

If the Δ found is much smaller than unity ($\Delta < 0.25$) or even negative, then it means that this method of solution is inadequate. When Δ is near unity, then this method should be effective. Therefore, the range of applicability of this method is established. Another advantage of this method is that the convergence can be certain. When the $\bar{Q}^*$ matches with the estimated $\bar{Q}$, it is equivalent to satisfying the set of N equations at the same time,

$$q_i : \text{Max } Y(q_i)\big|_{q_{j\neq i}}, \text{ for } i = 1, \ldots, N \qquad (3.1\text{-}10)$$

Lapidus [L.2] also proposed a direct search method similar to the pseudo-optimum method, except at the third step in the computational procedure, q_2^* is evaluated based on q_1^*, $q_3, \ldots, q_N$, instead of $q_1, q_3, \ldots, q_N$. Similarly for the rest of the q_i^*. This procedure will lead to two differences:

1. By using Lapidus' method, the next trial will automatically move to $q_1^*, q_2^*, \ldots, q_N^*$, while the pseudo-optimum method still has the choice of Δ value.
2. In Lapidus' method, the evaluation of q_i^* depends on $(q_1^*, \ldots, q_{i-1}^*, q_{i+1}, \ldots, q_N)$, while in the pseudo-optimum method, the q_i^* depend on $(q_1, \ldots, q_{i-1}, q_{i+1}, \ldots, q_N)$.

To illustrate the advantage of the pseudo-optimum method in regard to the first difference consider the following example: Assume the transformation functions of a multistage decision process to be

$$x_i = x_{i-1} + q_i \qquad (3.1\text{-}11)$$

$$y_i = y_{i-1} + (x_i - i)^2 \quad \text{for } i = 1, \ldots, 5 \qquad (3.1\text{-}12)$$

with the initial condition of

$$x_o = y_o = 0 \qquad (3.1\text{-}13)$$

The object function is the minimum of y_5. Denote y_5 by Y and it can be expressed as

$$Y = (q_1 - 1)^2 + (q_1 + q_2 - 2)^2 + (q_1 + q_3 - 3)^2 \qquad (3.1\text{-}14)$$
$$+ (q_1 + q_2 + q_3 + q_4 - 4)^2 + (q_1 + q_2 + q_3 + q_4 + q_5 - 5)^2$$

Obviously, the optimum solution is

$$q_1 = q_2 = q_3 = q_4 = q_5 = 1 \qquad (3.1\text{-}15)$$

which will give Y = 0. In order to compare two methods, let the initial estimate be

$$q_1 = q_2 = q_3 = q_4 = q_5 = 0 \qquad (3.1\text{-}16)$$

The corresponding value of Y is 55.

The algorithm as calculated by Lapidus' method is as follows:

1. Choose the optimal value of q_1, while q_2 through q_5 remain at their initial estimate. q_1 can be obtained from

$$\frac{\partial Y}{\partial q_1} = 0 \qquad (3.1\text{-}17)$$

We have

$$5\, q_1^* - 15 = 0$$

$$q_1^* = 3 \qquad (3.1\text{-}18)$$

2. Evaluate q_2^*, while the other decisions are

$$q_1 = 3,\ q_3 = 0,\ q_4 = 0,\ q_5 = 0 \qquad (3.1\text{-}19)$$

We obtain

$$\frac{\partial Y}{\partial q_2} = 4\ q_2 - 2 = 0 \qquad (3.1\text{-}20)$$

$$q_2^* = 0.5$$

3. Calculate q_3^* by the equation

$$\frac{\partial Y}{\partial q_3} = 0 \qquad (3.1\text{-}21)$$

where $q_1 = 3$, $q_2 = 0.5$, $q_4 = 0$, $q_5 = 0$. We obtain

$$q_3^* = 0.5 \qquad (3.1\text{-}22)$$

4. Similarly, we obtain

$$q_4^* = 0.5$$
$$q_5^* = 0.5 \qquad (3.1\text{-}23)$$

At the end of the first loop, the value of Y is 7.5

5. Iterate the loop.

The algorithm of the pseudo-optimum method for the same problem is as follows:

1. Choose the optimal value of q_1, while q_2 through q_5 remain at their initial estimation. We obtain

$$q_1^* = 3 \qquad (3.1\text{-}24)$$

2. Evaluate q_2^*, while q_1, q_3, q_4, q_5 remain at their initial estimated values, i.e.

$$q_1 = q_3 = q_4 = q_5 = 0 \qquad (3.1\text{-}25)$$

We have

$$\frac{\partial Y}{\partial q_2} = 4\ q_2 - 14 = 0 \qquad (3.1\text{-}26)$$

$$q_2^* = 3.5 \qquad (3.1\text{-}27)$$

3. Similarly, compute q_3^*, q_4^*, and q_5^*. They are

$$q_3^* = 4,\ q_4^* = 4.5,\ q_5^* = 5 \tag{3.1-28}$$

4. Calculate the new estimate as

$$q_i|_{new} = q_i|_{old} + (q_i^* - q_i|_{old}) \tag{3.1-9}$$

$$\text{for } i = 1, \ldots, 5$$

Substitute the original values for $q_1, \ldots, q_5$ and $q_1^*, \ldots, q_5^*$ into the above equations, we have

$$q_1 = 3\Delta,\ q_2 = 3.5\Delta,\ q_3 = 4\Delta,\ q_4 = 4.5\Delta,\ q_5 = 5\Delta \tag{3.1-29}$$

5. Again substitute these values into equation (3.1-14)

$$Y = (3\Delta - 1)^2 + (6.5\Delta - 2)^2 + (10.5\Delta - 3)^2 + (15\Delta - 4)^2 + (20\Delta - 5)^2 \tag{3.1-30}$$

The optimal value of Δ, which gives the minimum of Y, can be obtained by

$$\frac{\partial Y}{\partial \Delta} = 0 \tag{3.1-31}$$

Performing the operation on equation (3.1-30) gives

$$\Delta = 0.273$$

6. Using the optimal value of Δ, by equation (3.1-30), we have

$$Y = 0.323$$

7. Iterate the loop.

We note that at the end of first iteration, the value of Y obtained by the pseudo-optimum method is much less than that obtained by Lapidus' method. Another advantage of the pseudo-optimum method is that the evaluation of q_i^*'s is independent

of each other. Therefore, if the decisions are numerous, it becomes possible to evaluate only a few of these decisions, then interpolate to other decisions.

2. Numerical Example: Sequence of Stirred Tank Reactors

To illustrate the computational procedure of the pseudo-optimum method, a study was made to solve for the optimal temperature policy of the reaction A → B → C taking place in a sequence of three stirred tanks with equal residence times. The reaction A → B is of second order and the reaction B → C is of first order. The rate constants are of the form:

$$k_1 = A_1 \exp(-E_1/RT)$$
$$k_2 = A_2 \exp(-E_2/RT) \qquad (3.2\text{-}1)$$

The criterion of optimization is the maximum profit, which can be expressed as

$$Y = (b_3 - b_0) - \gamma (a_0 - a_3) \qquad (3.2\text{-}2)$$

where "a" and "b" denote the concentration of A and B, and the subscript indicates the number of the tank.

A similar problem was solved using iterative techniques by Denn and Aris [D.3]. The parameters assumed were

$A_1 = 5 \times 10^{10}$ liter/mole/min. $\quad E_1 = 18$ Kcal.

$A_2 = 3.33 \times 10^{17}$/min. $\quad E_2 = 30$ Kcal.

$\theta = 2$ min. (residence time) $\quad \gamma = 0.3$

$a_0 = 1$ mole/liter $\quad b_0 = 0$ mole/liter

Also, the temperature is assumed subject to the limits

$$T_L \leq T \leq T_U$$

where $T_L = 335^{\circ}K$ and $T_U = 355^{\circ}K$. The transformation functions

can be derived to be:

$$a_i = a_{i-1} - \theta\, k_1\, a_i^2 \quad \text{for } i = 1, 2, 3. \tag{3.2-3}$$

$$b_i = b_{i-1} + \theta\, k_1\, a_i^2 - \theta\, k_2\, b_i \quad \text{for } i = 1, 2, 3. \tag{3.2-4}$$

For a given temperature, a_i and b_i can be solved from equations (3.2-3) and (3.2-4) as

$$a_i = \frac{-1 + \sqrt{1 + 4\, a_{i-1}\, k_1\, \theta}}{2\, k_1\, \theta} \tag{3.2-5}$$

$$b_i = \frac{b_{i-1} + k_1\, a_i^2\, \theta}{1 + k_2\, \theta} \quad \text{for } i = 1, 2, 3. \tag{3.2-6}$$

The computational procedure by using the pseudo-optimum method is illustrated as follows:

1. Estimate the initial temperature in each tank. Denote by T_1, T_2, T_3.
2. Calculate the rate constants, k_1 and k_2, at the corresponding temperatures and evaluate outlet concentrations by the transformation equations.
3. Compute the profit by the formula

$$Y = b_3 - 0.3\,(1-a_3) \tag{3.2-7}$$

4. Within the range $335^{\circ}K \le T \le 355^{\circ}K$, find T_1^* by

$$T_1^* : \underset{T_1}{\text{Max}}\ Y\,(T_1, T_2, T_3)\,|\,T_2, T_3 \tag{3.2-8}$$

   The notation means T_1^* is the choice of T_1 which will give the maximum of Y, while T_2 and T_3 remain constant.
5. Similarly, find T_2^* and T_3^* by

$$T_2^* : \underset{T_2}{\text{Max}}\ Y\,(T_1, T_2, T_3)\,|\,T_1, T_3 \tag{3.2-9}$$

$$T_3^* = \underset{T_3}{\text{Max}}\ Y\ (T_1, T_2, T_3) | T_1, T_2 \qquad (3.2\text{-}10)$$

6. Take T_1^*, T_2^*, T_3^* as the new estimates, and repeat the cycle from step 2, until the difference between the estimated value and the corresponding pseudo-optimum temperatures is less than a tolerable error.

In this particular case difficulty is encountered in solving for T_i^*. The analytic solution is difficult or even impossible to obtain. Therefore, the one-dimensional search method can be used to find T_i^*.

There are several one-dimensional search methods available [W.1], such as dichotomous search, Fibonacci search, and Golden Section method. The last method was chosen for its effectiveness. The Golden Section Method follows a sequential search scheme. The first trial of T_1 is at

$$x_1 = T_L + \frac{T_U - T_L}{\tau} \qquad (3.2\text{-}11)$$

where T_L and T_U are the lower and upper limits, and τ = 1.618033989. Taking x_1 as the first stage temperature, and T_2 and T_3 as second and third stage temperatures, the profit can be evaluated as shown in step 2 and step 3. The second trial of T_1 is at

$$x_2 = T_L + R'/\tau^2 \qquad (3.2\text{-}12)$$

where

$$R' = T_U - T_L \qquad (3.2\text{-}13)$$

In a similar way, the profit can be found. Denote the profits of first and second trials by Y_1 and Y_2.

If Y_2 is less than Y_1 and x_2 is also less than x_1, then the optimal value of T_1 must be on the right hand side of x_2. Thus the lower limit is replaced by x_2. The third trial is located at

$$x_3 = T_U - R'/\tau^3 \qquad (3.2\text{-}14)$$

If Y_2 is less than Y_1, but x_2 is larger than x_1, then the optimum must be on the left hand side of x_2. The upper limit is replaced by x_2, and the third trial is located at

$$x_3 = T_L - R'/\tau^3 \qquad (3.21\text{-}15)$$

However, if $Y_2 > Y_1$ and $x_2 < x_1$, then the optimum will be on the left of x_1. x_1 takes place of upper limit, and the third trial will be at

$$x_3 = T_L + R'/\tau^3 \qquad (3.2\text{-}16)$$

If $Y_2 > Y_1$ and $x_2 > x_1$, then the optimum will be on the right of x_1. The lower limit is substituted by x_1 and the next trial is at

$$x_3 = T_U - R'/\tau^3 \qquad (3.2\text{-}17)$$

A flow chart of the algorithm is given in Figures 14 and 15. The procedure to obtain T_2^* and T_3^* is similar, except that the concentrations at the previous stage are fixed.

To prove the convergence of the pseudo-optimum method, the upper and lower limits were chosen to be the initial estimates. When the object program was run on the Osage computer [0.1], it took only 36 seconds. The results of two ascending series are given in Table 4. The temperature of successive trials is plotted in Figure 16. Figure 17 indicated a_3 versus b_3 in the two converging sequences.

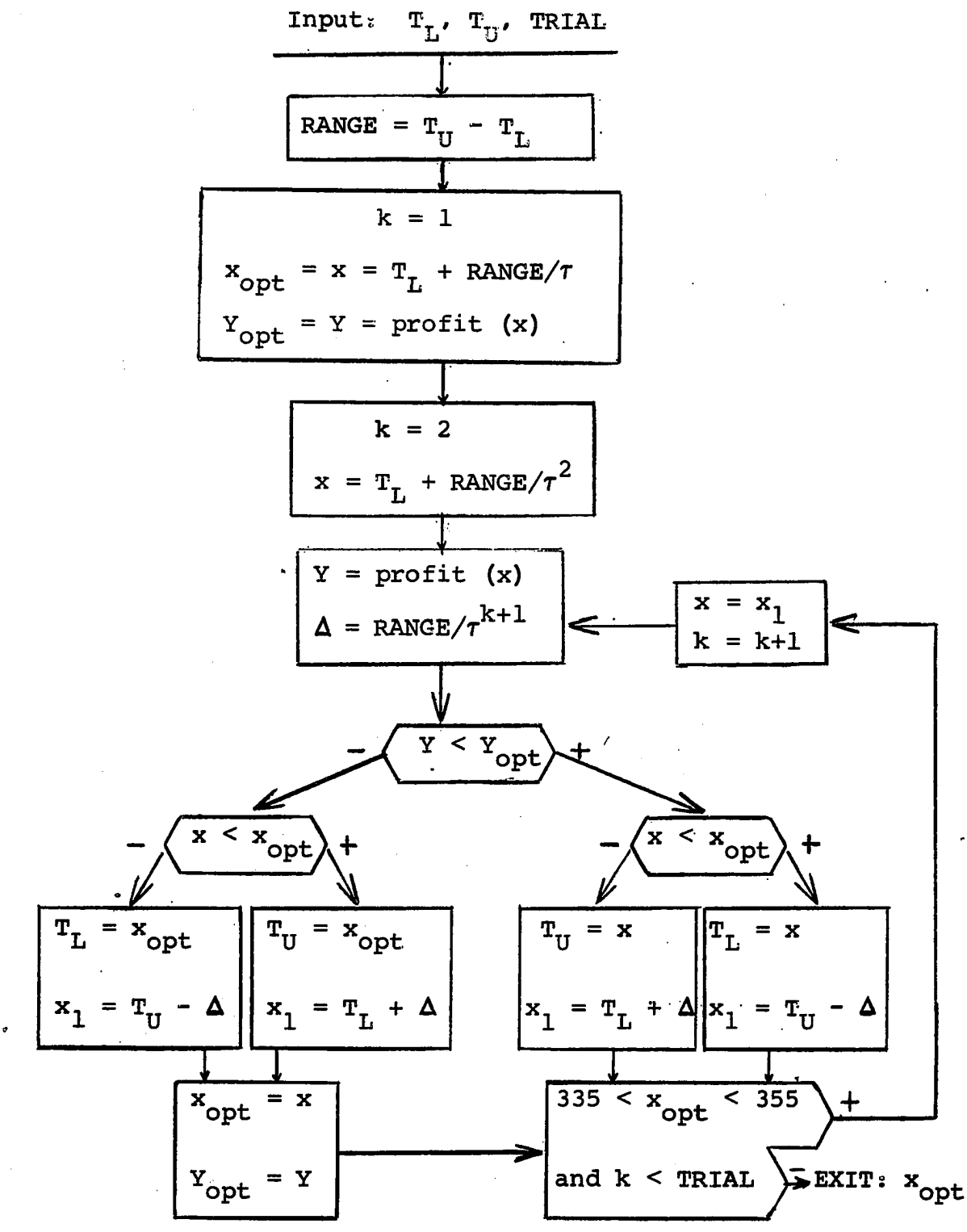


Figure 14. Flow Chart of One-Dimensional Search

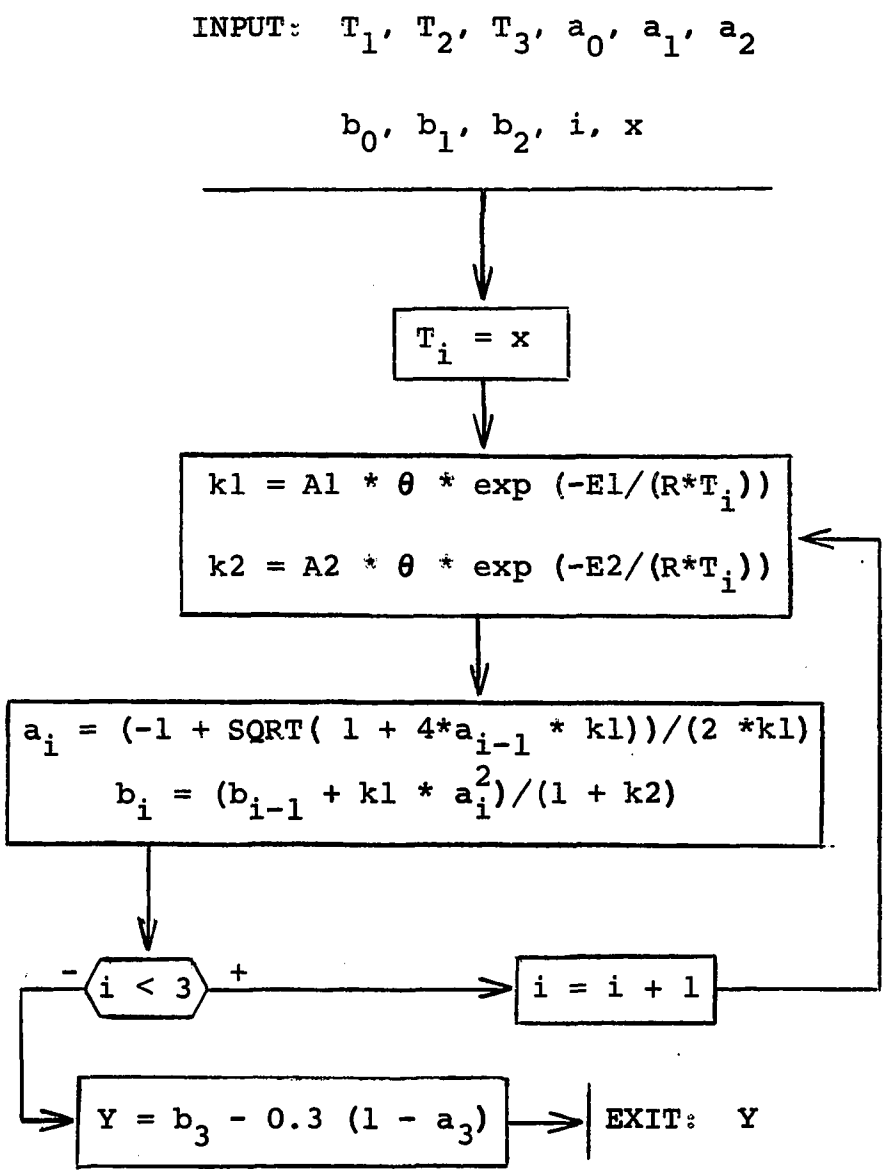


Figure 15. Flow Chart for Evaluation of Profit for a Given Set of Decisions

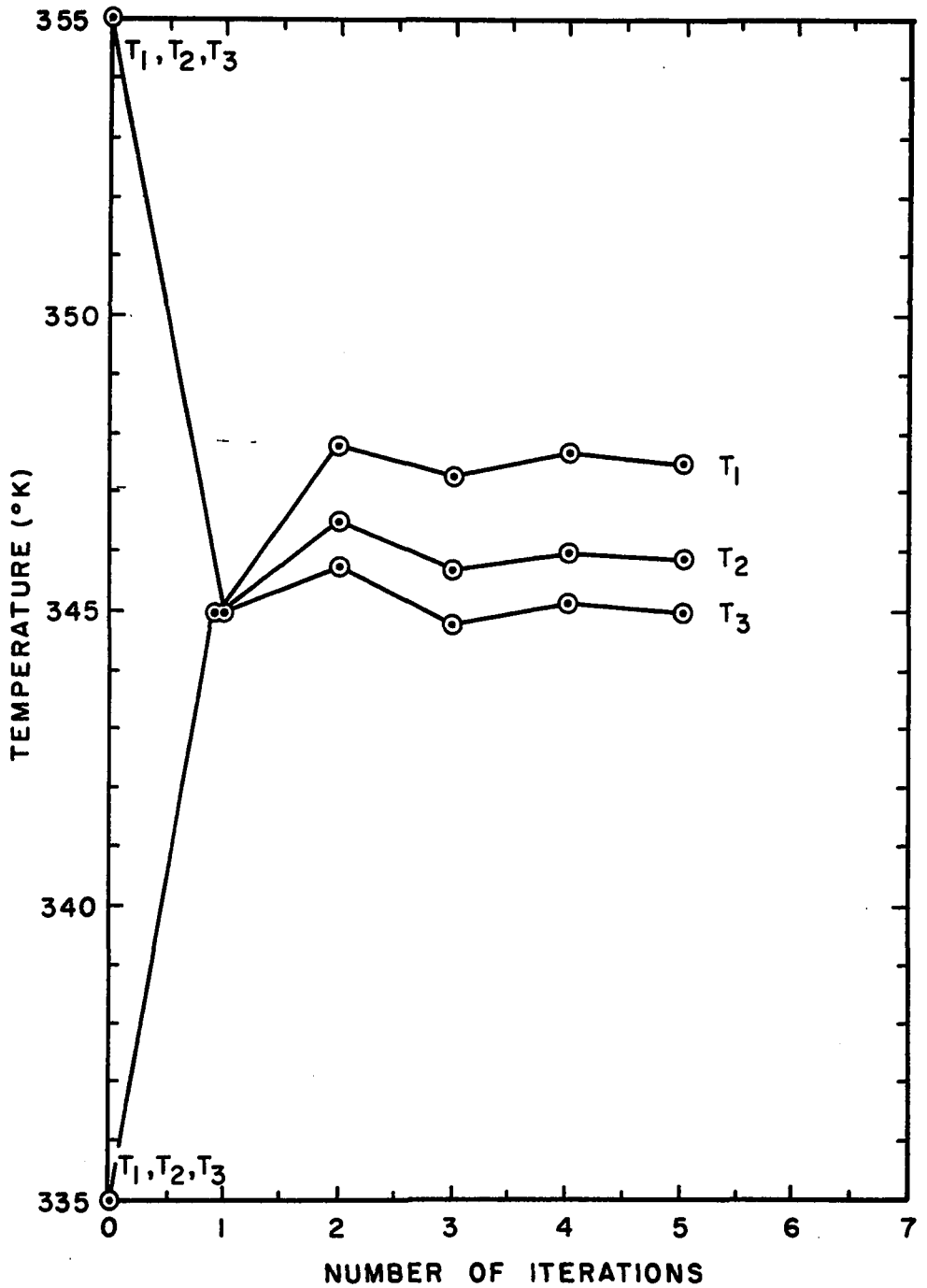


Figure 16.--Successive Approximation to Three Stage Temperature Policy

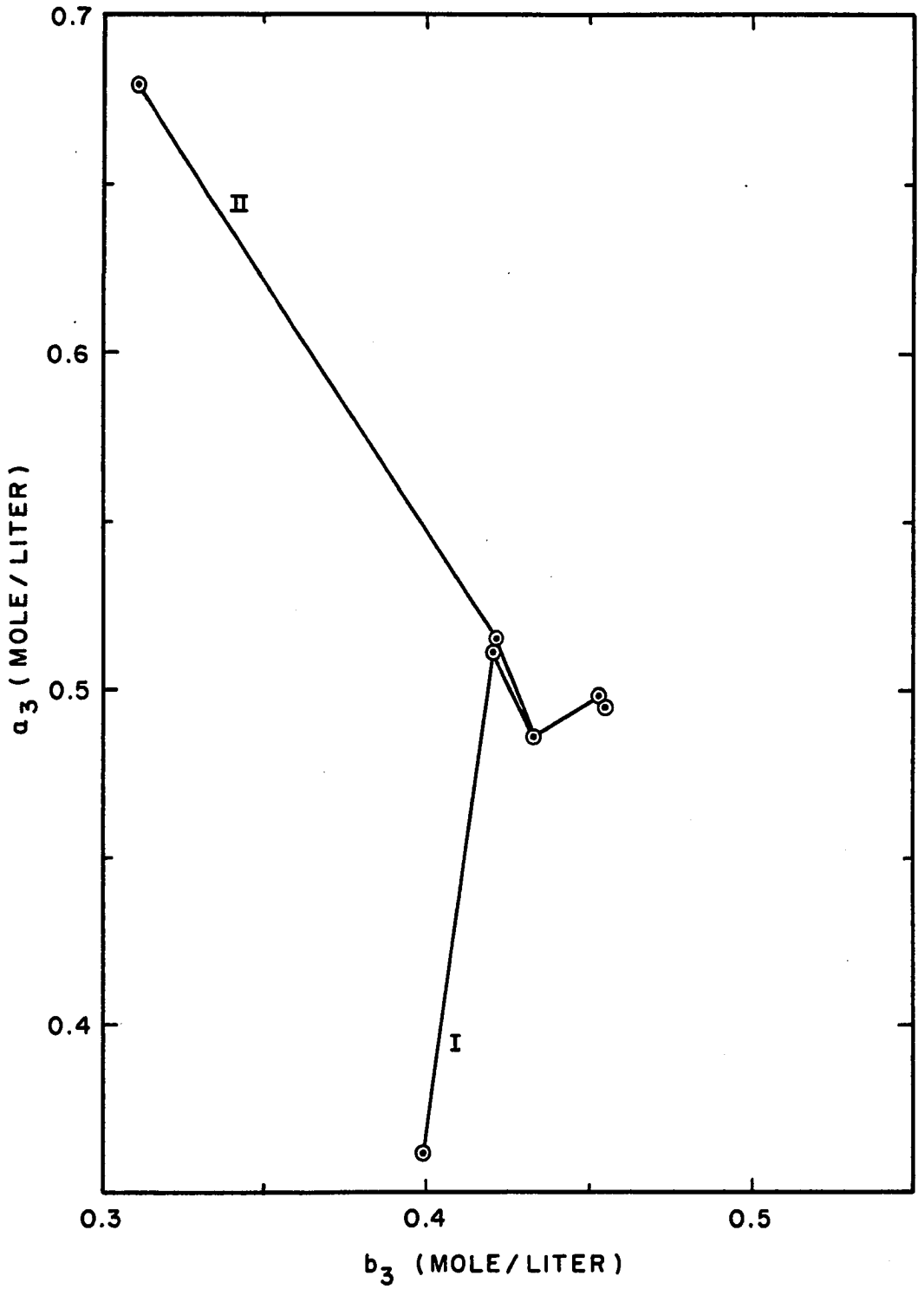


Figure 17.--Iteration Trajectories of Concentration a_3 and b_3

TABLE 4.

THE RESULTS OF TWO ASCENDING SERIES

Number of trial	T_1	T_2	T_3	a_3	b_3	Y
0	355.*	355.	355.	.361	.399	.20722
	335.#	335.	335.	.678	.310	.21348
1	345.03	345.03	345.03	.51248	.42234	.27609
	344.96	344.96	344.96	.51374	.42184	.27596
2	347.77	346.55	345.82	.48538	.43158	.27717
	347.81	346.59	345.86	.48472	.43172	.27714
3	347.24	345.69	344.85	.49801	.42796	.27736
	347.22	345.67	344.82	.49839	.42783	.27735
4	347.69	346.04	345.17	.49209	.42977	.27740
	347.67	346.06	345.18	.49194	.42982	.27740
Final	347.51	345.87	344.99	.49484	.42894	.27741

* : The first series. # : The second series.

3. Numerical Example: Absorption Tower

Consider the steady state of an absorption tower to be disturbed by a step change of input concentration. The system under the perturbation will move toward a new steady state. The problem becomes one of manipulating other input variables to minimize the time required to achieve a new steady state.

Lapidus and co-workers [L1, L3, L5] studied this problem and solved for the optimal input liquid concentration as a function of time. By using the pseudo-optimum method, it is possible to solve the optimal liquid flow rate for the same purpose. The model was first given by

Amundson and Lapidus [L.1]. A material balance around the i-th plate yields

$$L'(x_{i-1} - x_i) + G\,(y_{i+1} - y_i) = H'\frac{dy_i}{dt} + h\frac{dx_i}{dt} \tag{3.3-1}$$

where L' and G are the liquid and vapor flow rate respectively, h and H' are the liquid and vapor holdup respectively in each equilibrium plate, with x and y as concentrations of liquid and vapor phase. Using the equilibrium relation,

$$y_i = a'x_i + b' \tag{3.3-2}$$

we obtain

$$L'x_{i-1} - (L' + a'G)\,x_i + a'G\,x_{i+1} = (a'H' + h)\frac{dx_i}{dt} \tag{3.3-3}$$

Denote

$$d = L'\,G/a' \text{ and } e = \frac{a'H' + h}{a\,G} \tag{3.3-4}$$

the equation becomes

$$\frac{d\,x_i}{dt} = \frac{d}{e}x_{i-1} - \frac{d+1}{e}x_i + \frac{1}{e}x_{i+1} \text{ for } i = 1, \ldots, N \tag{3.3-5}$$

The boundary conditions are

$$x_i(t) = x_o, \text{ for } i = 0 \tag{3.3-6}$$

$$x_i(t) = (y_{N+1} - b)/a, \text{ for } i = N+1 \tag{3.3-6}$$

The initial conditions are

$$x_i\,(0) = x_i^o, \text{ for } i = 1, \ldots, N \tag{3.3-7}$$

The set of equations can be represented in matrix form:

$$\frac{d\,\bar{X}}{d\,t} = \bar{\bar{A}}\,\bar{X} + \bar{\bar{D}}\,\bar{M} \tag{3.3-8}$$

where

$$\bar{\bar{A}} = \begin{bmatrix} -\frac{d+1}{e} & \frac{1}{e} & 0 & 0 & 0 \\ \frac{d}{e} & -\frac{d+1}{e} & \frac{1}{e} & 0 & 0 \\ 0 & \frac{d}{e} & -\frac{d+1}{e} & \frac{1}{e} & 0 \\ 0 & 0 & .. & ... & .. \\ 0 & 0 & 0 & ..... & \end{bmatrix} \qquad (3.3\text{-}9)$$

$$\bar{\bar{D}} = \begin{bmatrix} \frac{d}{e} & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & \frac{1}{e} \end{bmatrix} \quad \bar{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} \quad \bar{E} = \begin{bmatrix} x_o \\ \frac{y_{N+1} - b'}{a'} \end{bmatrix} \qquad (3.3\text{-}10)$$

The solution of the matrix differential equation was obtained by Lapidus, as

$$\bar{X}(t) = e^{\bar{\bar{A}} t} \bar{X}(0) + \int_0^t e^{\bar{\bar{A}} t - s} \bar{\bar{D}} \cdot \bar{E} \, ds \qquad (3.3\text{-}11)$$

Suppose that the input condition is changed by a series of step functions, then

$$\bar{X}(t_k) = \bar{\bar{\Phi}} \bar{X}(t_{k-1}) + \bar{\bar{\Delta}} \cdot \bar{E}(t_{k-1}) \qquad (3.3\text{-}12)$$

where

$$\bar{\bar{\Phi}} = e^{\bar{\bar{A}} (t_k - t_{k-1})} \qquad (3.3\text{-}13)$$

$$= \bar{\bar{I}} + \bar{\bar{A}} (t_k - t_{k-1}) + \frac{\bar{\bar{A}}}{2!} (t_k - t_{k-1})^2 + \frac{\bar{\bar{A}}}{3!} (t_k - t_{k-1})^3 + \ldots$$

$$\bar{\bar{\Delta}} = \bar{\bar{D}} \cdot \int_{t_{k-1}}^{t_k} e^{\bar{\bar{A}} s} \, ds \qquad (3.3\text{-}14)$$

$$= \bar{\bar{D}} \cdot (t_k - t_{k-1}) \left[\bar{\bar{I}} + \frac{\bar{\bar{A}}(t_k - t_{k-1})}{2!} + \frac{\bar{\bar{A}}^2 (t_k - t_{k-1})^2}{3!} + \cdots \right]$$

$\bar{\bar{I}}$ is a unit matrix. Let the total outlet concentration disturbance be expressed by

$$\int_o^\infty (x_N(t) - x_f)^2 \, dt \qquad (3.3\text{-}15)$$

where x_f is the outlet concentration at the final steady state. Denote the integration by Y. Y can be approximated by

$$Y = \sum_{i=1}^{M} (x_N(t_i) - x_f)^2 \, (t_i - t_{i-1}) \qquad (3.3\text{-}16)$$

where M is a large number. In general, Y depends on x_N. By equation (3.3-12), x_N is function of the matrices $\bar{\bar{A}}$, $\bar{\bar{D}}$, and $\bar{E}$ which are again related to d, e and x_o . d and e were defined as

$$d = \frac{L'G}{a'} \text{ and } e = \frac{a' H + h}{a' G} \qquad (3.3\text{-}17)$$

Among these factors, only the input liquid concentration, x_o, and input flow rate, L, are likely subject to control. Lapidus solved for optimal x_o, which will give the minimum Y. However, it is easier to manipulate the flow rate than the concentration. So we consider the criterion of optimization to be the minimum of Y by manipulating the absorbent flow rate, L'(t). Note that L'(t) is not just a single variable, but a functional. In a discrete sense, L'(t) can be expressed as

$$L'(t) = L'_1 \text{ for } t_o \leq t < t_1$$

$$L'(t) = L'_i \text{ for } t_{i-1} \leq t \leq t_i \qquad (3.3\text{-}18)$$

....

$$L'(t) = L'_o \text{ for } t_M < t$$

where L_o is the initial as well as final flow rate. Now this problem can be reduced to the standard form as

$$Y = Y\ (L'_1, \ \ldots, \ L'_M) \qquad (3.3\text{-}19)$$

The necessary condition of optimization is

$$L'_i : \ \text{Min } Y\ (L'_i)\big|_{L'_{j\neq i}} \ , \text{ for } i = 1, \ \ldots, \ M \qquad (3.3\text{-}20)$$

which means that while the flow rate in other time periods remains unchanged, the flow rate L'_i during the time period

$$t_{i-1} \leq t < t_i \qquad (3.3\text{-}21)$$

should be chosen to make the disturbance, Y, the least.

The parameter values given by Lapidus as

N	= 6 plates	h	= 75 lb.
L'_o	= 40.8 lb./min	a'	= 0.72
G	= 66.7 lb./min.	b'	= 0
H'	= 1 lb.	x_o	= 0

The initial conditions were

$X_0(0) = 0$	$x_4(0) = 0.1954247$
$x_1(0) = 0.0613266$	$x_5(0) = 0.2274376$
$x_2(0) = 0.1134541$	$x_6(0) = 0.2546465$
$x_3(0) = 0.1577626$	$y_7(0) = 0.2$

The disturbance was a step increase of

$$y_7(t) = 0.3 \text{ for } t > 0$$

The corresponding final absorbent concentration leaving the tower was

$$x_f = 0.38197$$

In order to prevent the absorption tower from flooding or entraining liquid, upper and lower bounds are set on the liquid flow rate. Then for a given set values of L_1^i, ..., L_M^i, Y can be evaluated. The computational procedure for obtaining the optimum of L_1^i, ..., L_M^i is similar to that of previous section. Figures 18, 19 and 20 give the discrete optimal flow rate profiles versus time for allowable variation of 20%, 40% and 100% respectively in the liquid flow rate. Figure 21 shows the outlet concentration versus time for the three cases and for the standard case of flow rate remaining constant.

Figure 21 indicates that the larger the liquid flow rate range allowed, the faster the outlet concentration converges to its final state. Nonetheless, the response time (time required for the response to come within ±5 percent of its ultimate value) is six minutes in the case of 20% allowable variation on flow rate, which is about the same as by manipulating the inlet liquid concentration [L.3].

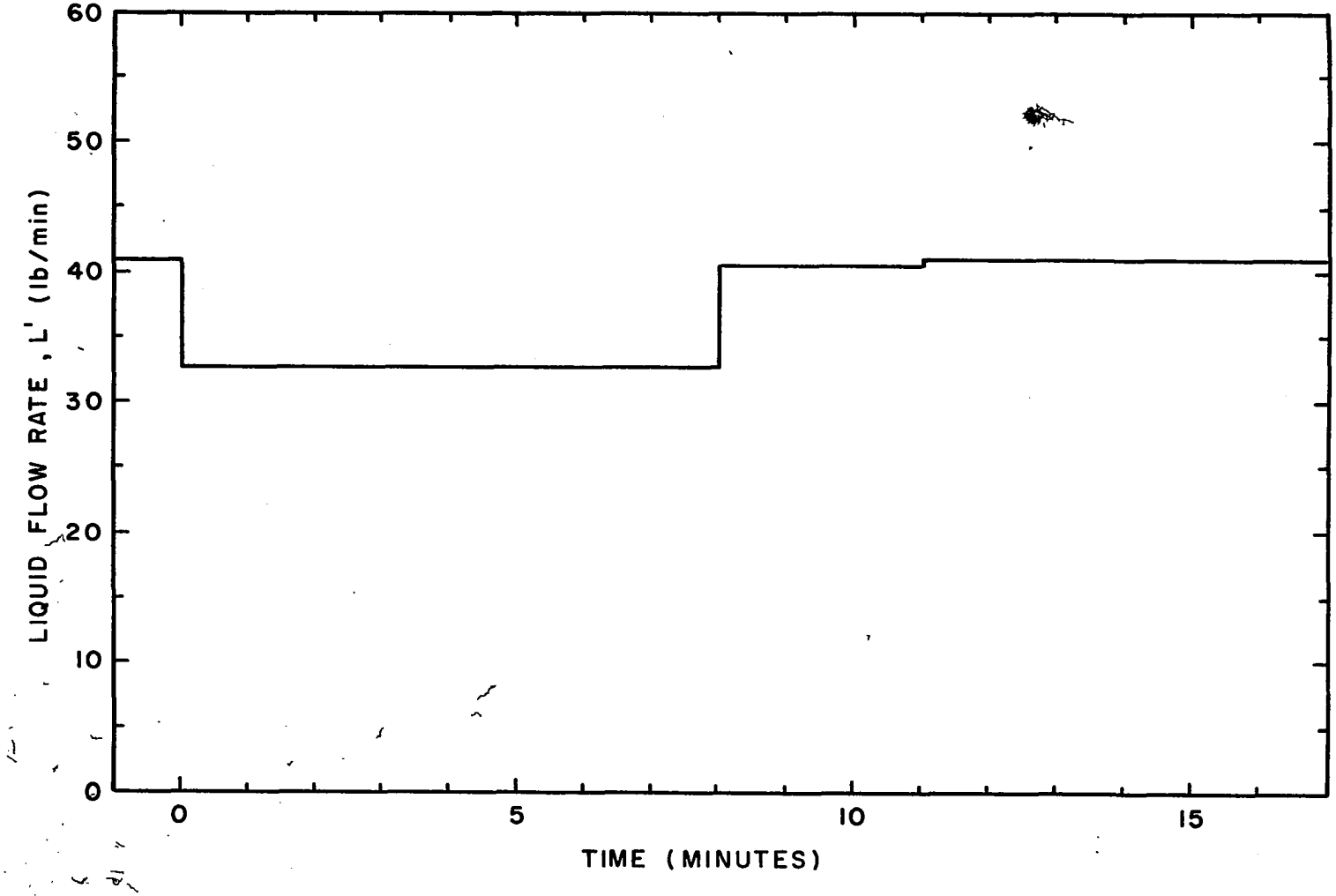


Figure 18.--Discrete Optimal Liquid Flow Rate L' versus Time for a Maximum Allowable Variation of 20%

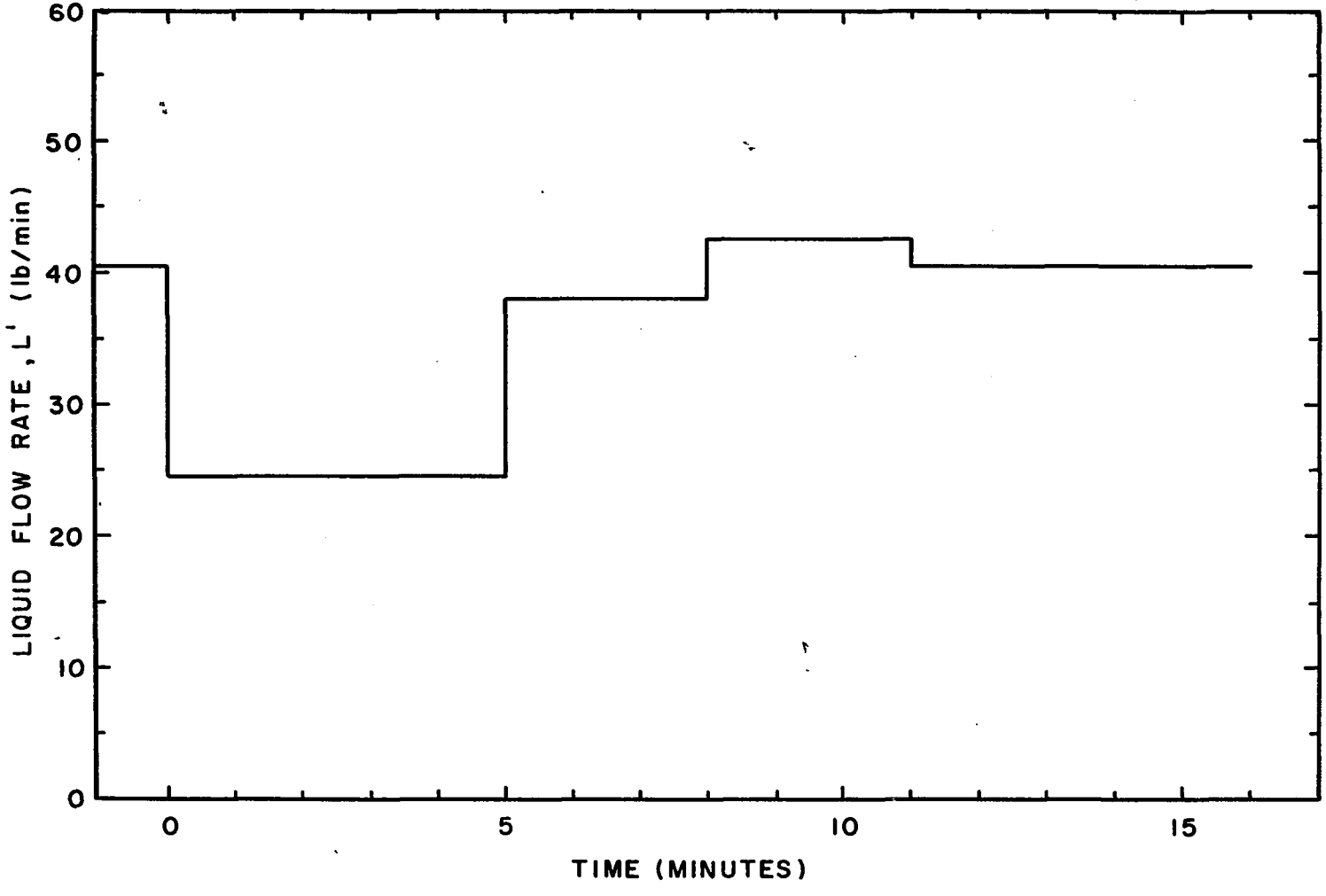


Figure 19.--Discrete Optimal Liquid Flow Rate, L', versus Time for a Maximum Allowable Variation of 40%

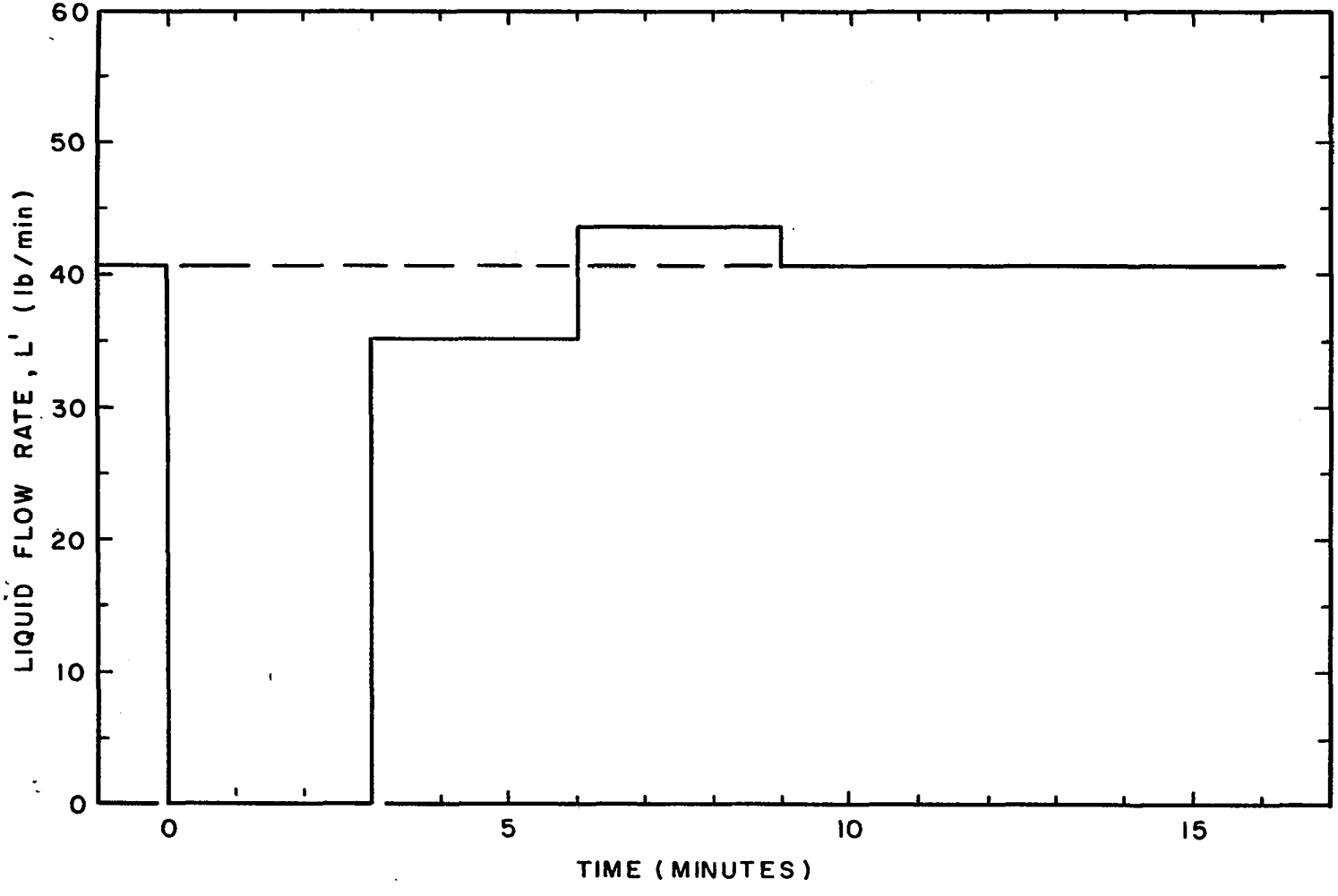


Figure 20.--Discrete Optimal Liquid Flow Rate, L', versus Time for a Maximum Allowable Variation of 100%

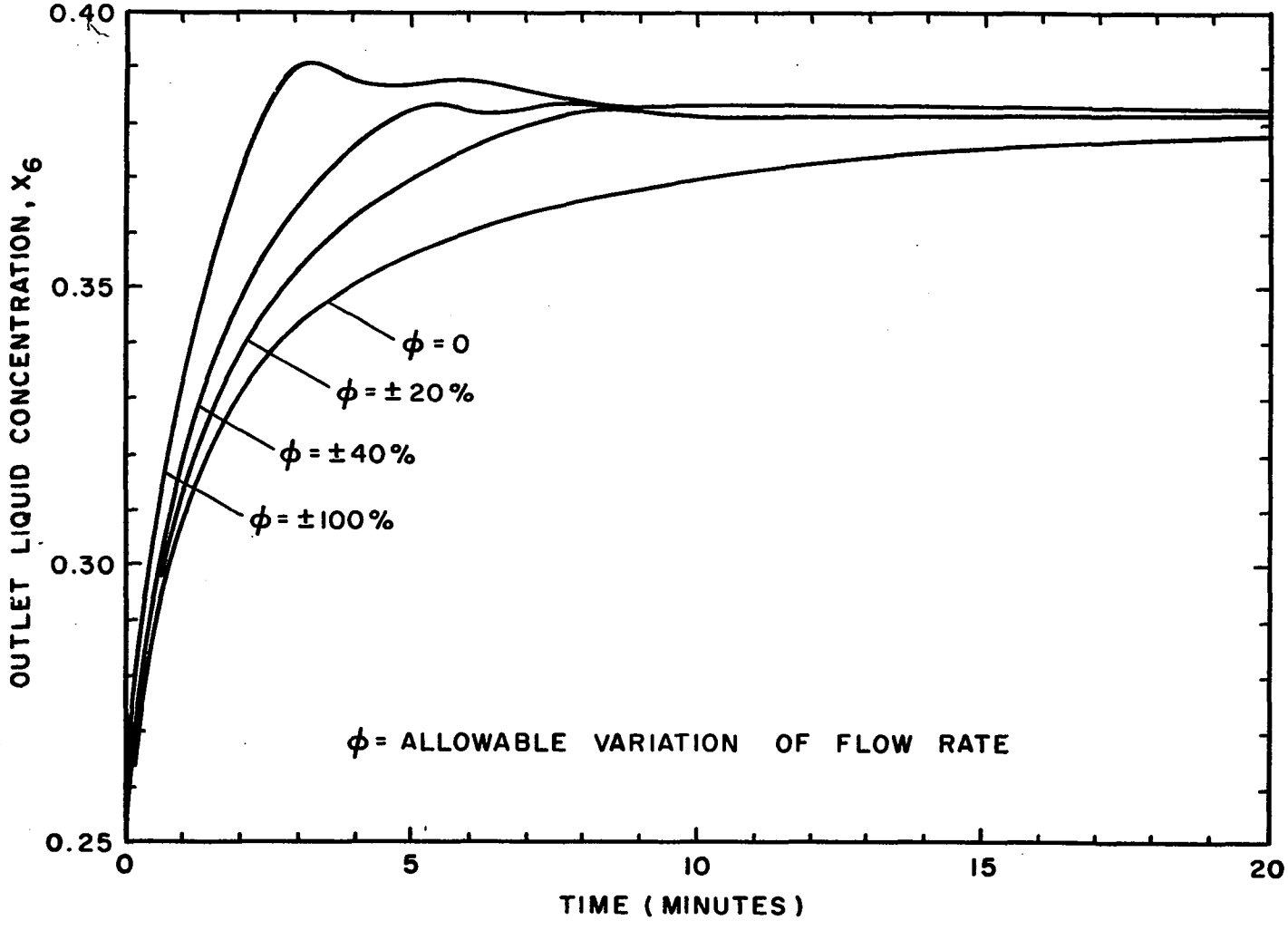


Figure 21.--The Transient Response of Outlet Liquid Concentration, x_6, for Six Tray Absorption Column

CHAPTER IV

OPTIMIZATION OF A TWO-DIMENSIONAL TUBULAR REACTOR

1. Previous Work

Since the chemical reactor always plays an important role in chemical engineering, the optimization of the reactor has received much attention. The optimum reaction temperature for a reversible, exothermic reaction was first derived by Denbigh [D2] in 1944 and is

$$T_{opt} = \frac{T_{eq}}{1 + \frac{R\,T_{eq}}{E_2 - E_1} \ln(E_2/E_1)} \qquad (4.1\text{-}1)$$

where T_{opt} and T_{eq} are the optimal temperature and the equilibrium temperature, respectively. E_1 and E_2 are the corresponding activation energies of synthesis and decomposition.

The theory of the existence of optimum temperature has been applied by various authors; Annable [A1] compared the conversion for the optimum temperature profile in the synthesis of ammonia with conversion for the actual temperature profile in an existing plant which compare as 22.9% and

and 19.29%. In other words, it might be possible to increase the yield by 18.7%.

Calderbank [C.1] calculated that with an optimum temperature profile the rate of oxidization of SO_2 to a certain conversion level of H_2SO_4 could increase 373%, compared with an externally cooled catalyst bed. Kuckler [K.3] set the best temperature for an isothermal tubular reactor and predicted the optimum distribution of catalyst and inlet temperature for two adiabatic reactors in series.

More important and systematic works were developed or collected by Aris [A.2] in the book "The Optimum Design of Chemical Reactor." By means of dynamic programming, he derived the optimal temperature policy for a tubular reactor with a single reversible reaction, consecutive reactions, and simultaneous reactions. However, the models of a tubular reactor are based on the plug flow assumption, which is a homogenous flow with axial uniformity. Because the reaction rate is an exponential function of temperature, the neglect of radial temperature and concentration gradient will cause serious error in the case of fixed bed catalytic reactor. Aris also recognized that the optimum temperature policy he derived could not be realized in practice [A.3].

Gray [G.1, G.2] made a study on the optimal wall heat flux profile so as to maximize the final conversion of a first order, reversible, exothermic reaction in a two-dimensional tubular reactor model. He considered that the extent of reaction, c, and the dimensionless temperature,

T, in a packed bed reactor could be represented by following equations

$$\frac{\partial c}{\partial z} = \frac{s}{Pe}\frac{1}{r}\left(r\frac{\partial}{\partial r}\frac{\partial c}{\partial r}\right) + Da_I\, R(c,T) \qquad (4.1\text{-}2)$$

$$\frac{\partial T}{\partial z} = \frac{s}{Pe'}\frac{1}{r}\left(r\frac{\partial}{\partial r}\frac{\partial T}{\partial r}\right) + Da_{III}\, R(c,T) \qquad (4.1\text{-}3)$$

where s is the ratio of length to radius. Pe and Pe' are the radial Peclet numbers for mass diffusion and heat transfer, respectively. z and r are dimensionless axial and radial distance. R(c,T) is the dimensionless reaction rate, defined as

$$R(c,T) = (1-c)\, e^{E_1(1-1/T)} - ce^{E_{02}-E_2/T} \qquad (4.1\text{-}4)$$

Da_I and Da_{III} are the first and third Damkohler numbers:

$$Da_I = LR_o/V \qquad (4.1\text{-}5)$$

$$Da_{III} = Da_I\, \Delta H/(\rho C_p T_o') \qquad (4.1\text{-}6)$$

where L and V are the axial length and velocity respectively. R_o is the actual reaction rate which occurs when the dimensionless temperature is unity and the extent of reaction is zero. T_o refers to the absolute temperature on which the dimensionless temperature is based.

Boundary conditions for the differential equations are

$$c(r,0) = c_{in}, \qquad T(r,0) = T_{in}$$

$$\frac{\partial c}{\partial r} = 0, \qquad \frac{\partial T}{\partial r} = 0 \text{ at } r = 0$$

$$\frac{\partial c}{\partial r} = 0, \qquad \frac{\partial T}{\partial r} = -Q(z) \text{ at } r = 1 \qquad (4.1\text{-}7)$$

$Q(z)$ is the dimensionless wall heat flux, defined as

$$Q(z) = qL/(sh_T T_o) \qquad (4.1\text{-}8)$$

where q is the heat flux rate per unit area, and h_T is the heat transfer coefficient.

The numerical method for solving these equations was given by Mickley and Letts [M.2]. The method is to reduce the partial differential equations to the following differential difference approximations:

$$\frac{dc_o}{dz} = \frac{s\,M^2}{Pe}\,4(c_o - c_1) + Da_I R(c,T) = g_o$$

$$\frac{dc_i}{dz} = \frac{s\,M^2}{Pe}\left(\frac{2i+1}{2i}\,c_{i+1} - 2c_i + \frac{2i-1}{2i}\,c_{i-1}\right) + Da_I R(c_i,T_i) = g_i$$

$$\text{for } i = 1, 2, \ldots, M-1$$

$$\frac{dc_M}{dz} = \frac{s\,M^2}{Pe}\,(c_{M-1} - c_M) + Da_I R(c_M,T_M) = g_M \qquad (4.1\text{-}9)$$

and

$$\frac{dT_o}{dz} = \frac{s\,M^2}{Pe}\,4(T_o - T_1) + Da_{III} R(c_o, T_o) = h_o$$

$$\frac{dT_i}{dz} = \frac{s\,M^2}{Pe'}\left(\frac{2i+1}{2i}\,c_{i+1} - 2c_i + \frac{2i-1}{2i}\,c_{i-1}\right) + Da_{III}R(c_i,T_i) = h_i$$

for i = 1, 2, ..., M-1

$$\frac{dT_M}{dz} = \frac{s\,M^2}{Pe'}\,(T_{M-1}-T_M) - (2M+1)\,\frac{sQ}{Pe'} + Da_{III}R(c_M,T_M) = h_M \qquad (4.1\text{-}10)$$

where M is the total number of radial increments.

The gradient technique of Bryson, which was reviewed in Chapter I, was used by Gray to find the optimal heat profile. The adjoint equations become:

$$\frac{dD_{c_o}}{dz} = -D_{c_o}\frac{\partial g_o}{\partial c_o} - D_{c_o}\frac{\partial g_o}{\partial c_o}\,D_{T_o}\frac{\partial h_o}{\partial c_o}$$

$$\frac{dD_{c_i}}{dz} = -D_{c_{i-1}}\frac{\partial g_{i-1}}{\partial c_{i-1}} - D_{c_i}\frac{\partial g_i}{\partial c_i} - D_{c_{i+1}}\frac{\partial g_{i+1}}{\partial c_{i+1}} - D_{T_i}\frac{\partial h_i}{\partial c_i}$$

for i = 1, 2, ..., M-1

$$\frac{dD_{c_N}}{dz} = -D_{c_{M-1}}\frac{\partial g_{M-1}}{\partial c_{M-1}} - D_{c_M}\frac{\partial g_M}{\partial c_M} - D_{c_M}\frac{\partial h_M}{\partial c_M} \qquad (4.1\text{-}11)$$

$$\frac{dD_{T_o}}{dz} = -D_{T_o}\frac{\partial h_o}{\partial T_o} - D_{T_i}\frac{\partial h_i}{\partial T_o} - D_{c_o}\frac{\partial g_o}{\partial T_o}$$

$$\frac{dD_{T_i}}{dz} = -D_{T_{i-1}}\frac{\partial h_{i-1}}{\partial T_i} - D_{T_i}\frac{\partial h_i}{\partial T_i} - D_{T_{i+1}}\frac{\partial h_{i+1}}{\partial T_i} - D_{T_i}\frac{\partial g_i}{\partial T_i}$$

for i = 1, ..., M-1

$$\frac{dD_{T_N}}{dz} = -D_{T_{N-1}} \frac{\partial h_{N-1}}{\partial T_N} - D_{T_N} \frac{\partial h_N}{\partial T_N} - D_{C_N} \frac{\partial g_N}{\partial T_N} \qquad (4.1\text{-}12)$$

The boundary conditions at z = 1 are as follows:

$$D_{C_o} = 0$$

$$D_{C_i} = \frac{2i}{M^2} \text{ for } i = 1, \ldots, M - 1 \qquad (4.1\text{-}13)$$

$$D_{C_N} = 1/N$$

$$D_{T_i} = 0 \text{ for } i = 1, \ldots, M - 1 \qquad (4.1\text{-}14)$$

The computation scheme is as follows:

1. Estimate a heat flux profile and evaluate the concentration and temperature distribution through the two-dimensional reactor by the method given by Letts and Mickley.
2. Integrate the adjoint function from the exit to the inlet.
3. Change the heat flux in proportion to $-D_{T_M}(z)$, i.e.

$$Q(z)\big|_{new} = Q(z)\big|_{old} - \Delta\, D_{T_M}(z)$$

for z = 0 to z = 1

where Δ is a constant.

4. Repeat the cycle. If the yield is less than the previous trial then halve the value of Δ. Iterate the loop until Δ is very small.

Starting from two distinct estimations, Gray obtained two different final profiles. Obviously, the method failed

in at least one of the cases. As a matter of fact, the conversions at the end of two series of ascents are 0.1442 and 0.14483, but the best yield obtainable is 0.15062.

2. Fixed Bed Reactor Model

There are two categories of models to represent a fixed bed chemical reactor. In the first category a set of partial differential equations describing the mass diffusion and the heat transfer are used. General formulas are as follows:

$$\frac{\partial C}{\partial t} + \bar{V}\cdot\nabla C = \nabla\cdot(\bar{K}'\cdot\nabla C) + r_c \qquad (4.2\text{-}1)$$

$$\frac{\partial T}{\partial t} + \bar{V}\cdot\nabla T = \nabla\cdot(\bar{K}\cdot\nabla T) + r_c\Delta H \qquad (4.2\text{-}2)$$

where $\bar{V}$ is the velocity vector. $\bar{K}'$ and $\bar{K}$ are dispersion coefficients for mass and heat transfer; r_c is the chemical conversion rate. Although numerical methods can be used to solve the set of partial differential equations, the boundary conditions as well as the kinetic equations will cause the scheme to be very complicated. Therefore, some assumptions or simplifications are usually made. A few different approaches are given in the following discussion.

In 1946 Grossman [G.3] presented a double stepwise method of integration to evaluate the temperature profile in a cylindrical reactor in both axial and radial direction. He used the average temperature and concentration in each small but finite increment to calculate the corresponding reaction rate.

Singer and Wilhelm [S.1] in 1950 assumed non-existence of axial heat conduction and axial mass diffusion and then the temperature and concentration profiles in a cylindrical case were solved. The reaction rate was treated independent of concentration but as a function of temperature.

The mathematical model used by Carberry [C.2] contains such factors as the axial mixing, the effect of volume change, the temperature and concentration gradient between particles and the fluid as well as the diffusion inside a porous catalyst. However, the gradient of mass and heat in the radial direction was neglected.

Another category is the so-called tanks-in-series models. Either one-dimensional or two-dimensional series of perfectly mixed tank reactors are designated to represent the actual tubular fixed bed reactor. As shown in Figure 22, Deans and Lapidus [D.1] suggested the division of the tubular reactor into two-dimensional arrays of perfect stirred tanks with both width and length equal to one particle diameter. Different distances across the radius were chosen to make it correspond to the real diffusion effect. Upon the assumptions of (1) fully developed turbulent flow in the external field, (2) axially symmetric, (3) negligible series contribution to the heat transfer which includes the convection from the fluid to the particle surface, the conduction through the porous particles and radiation, (4) constant values of the transport coefficients. The following dynamic response of concentration at (i,j)th stage

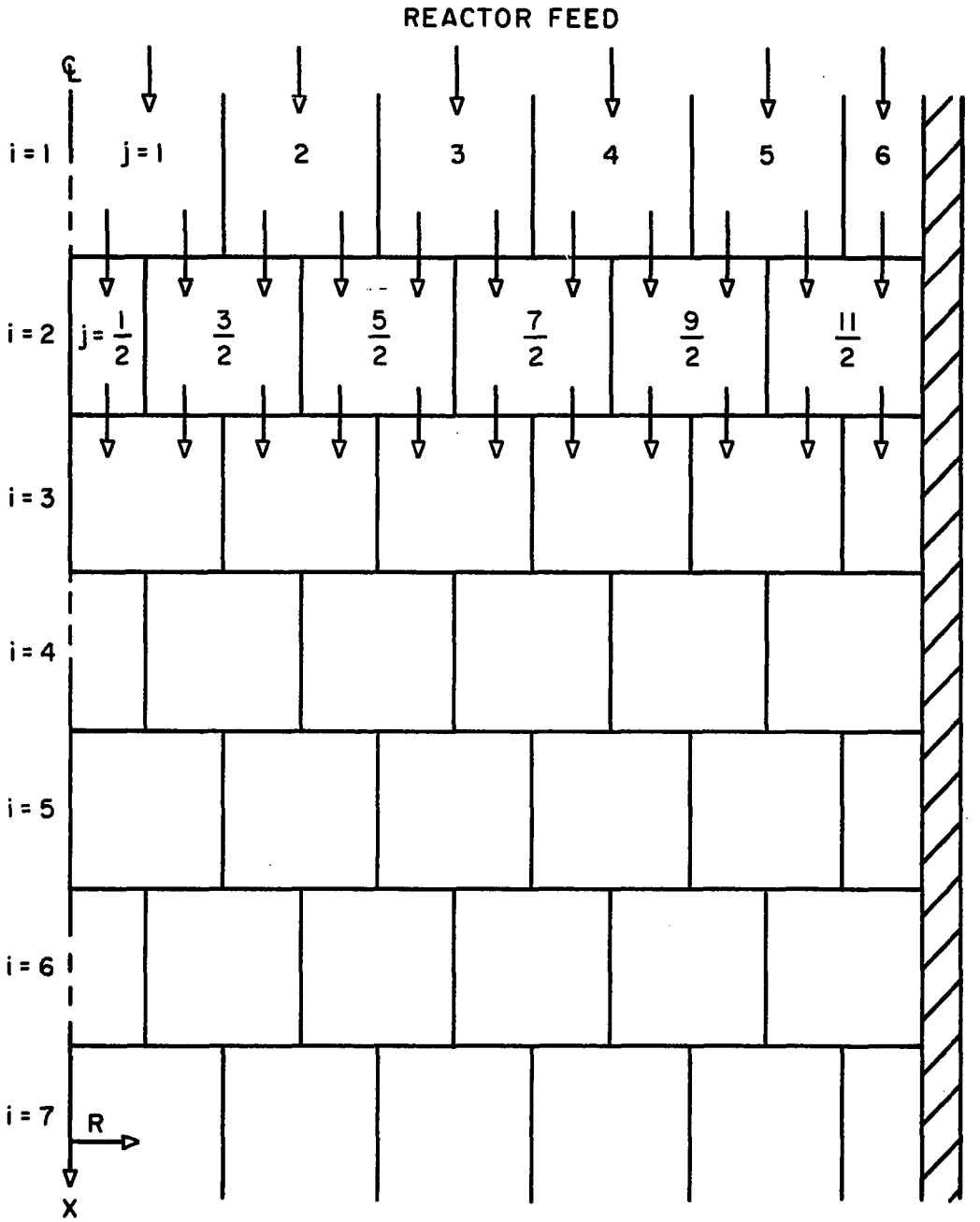


Figure 22.--Two-Dimensional Reactor, showing how Mixing Mechanism Occurs

can be obtained by material balance:

$$\xi\nu \frac{dC_{ij}}{dt} = Q'_{ij}(\varphi_{i-1,j} - C_{i,j}) + (\text{transfer from particle}) \tag{4.2-3}$$

for i = 1, ..., N and j = 1, ..., M, where ξ is the ratio of fluid volume to total volume, ν is the volume, Q' is the flow rate, and φ is the weight average feed to the (i,j) stage from the previous stage. If we further assume constant flow velocity, V, and steady state, then we have

$$c_{i,j} = R_{i,j} + \varphi_{i-1,j} \tag{4.2-4}$$

$$\text{for } i = 1, \ldots, N, \text{ and } j = 1, \ldots, M$$

where

$$R_{i,j} = \left(\begin{matrix}\text{Mass transfer} \\ \text{from particle}\end{matrix}\right) / Q'_{i,j}$$

$$= \frac{r_c \left(\begin{matrix}\text{Cross section} \\ \text{of the stage}\end{matrix}\right) L/N}{\left(\begin{matrix}\text{Cross section} \\ \text{of the stage}\end{matrix}\right) V}$$

$$= \frac{r_c L}{NV} \tag{4.2-5}$$

$$\varphi_{i-1,j} = \frac{(j-3/4)\ c_{i-1,j-\frac{1}{2}} + (j-\frac{1}{4})\ c_{i-1,j+\frac{1}{2}}}{(2j-1)} \tag{4.2-6}$$

r_c denotes the mass transfer rate per unit volume from a particle. Similar relations hold for the temperature distribution

$$T_{i,j} = P'_{i,j} + \psi_{i-1,j}, \text{ for } \begin{matrix} i=1, \ldots, N \\ j=1, \ldots, M \end{matrix} \tag{4.2-7}$$

where

$$P'_{i,j} = \left(\begin{matrix}\text{heat transfer}\\ \text{from particle}\end{matrix}\right)/(Q'\rho C_p)_{i,j} \qquad (4.2\text{-}8)$$

$$\psi_{i-1,j} = \frac{(j-.75)T_{i-1,j-\frac{1}{2}} + (j-\frac{1}{4})T_{i-1,j+\frac{1}{2}}}{(2j-1)} \qquad (4.2\text{-}9)$$

For a non-adiabatic reactor, there is heat exchange at wall stages where the steady state temperature equation becomes

$$T_{i,M} = \psi_{i-1,M} + S'_i + P'_{i,M} \text{ for } i = 1, \ldots, N \qquad (4.2\text{-}10)$$

where

$$S'_i = \left(\begin{matrix}\text{heat transfer}\\ \text{from the wall}\end{matrix}\right)/(Q'\rho C_p)_{i,M} \qquad (4.2\text{-}11)$$

The flow rate in a full stage is

$$Q' = (2M-1)\pi V d_p^2 \qquad (4.2\text{-}12A)$$

In a half stage the flow rate is

$$Q' = (M-\tfrac{1}{4})\pi V d_p^2 \qquad (4.2\text{-}12B)$$

The heat transfer rate from the wall is equal to the heat flux rate per unit area, q, multiplied by the contacted wall surface, A, where

$$A = 2\pi M d_p \cdot L/N \qquad (4.2\text{-}13)$$

$$d_p = (\text{diameter of reactor})/2M = R_t/M \qquad (4.2\text{-}14)$$

So that if we define the Stanton number by

$$N_{st} = \frac{2M^2}{(2M-1)N} \quad \text{for full stage} \tag{4.2-15A}$$

$$N_{st} = \frac{2M^2}{(M-\frac{1}{4})N} \quad \text{for half stage} \tag{4.2-15B}$$

and dimensionless heat flux, Q, by

$$Q = \frac{q \cdot L}{VC_p\rho \cdot R_t} \tag{4.2-16}$$

then

$$S_i' = Q_i N_{st} \tag{4.2-17}$$

Dean and Lapidus found that this model--consisting of N x M perfect stirred tanks with both width and length of each full stage equal to one particle diameter--would correspond to a fixed bed with an average radial Peclet number equal to 8.2 and axial Peclet number equal to 2.0. However, by changing the size of stages, it can be made analogous to any experimental result. The adjusted stage size will be

$$\text{Width} = \sqrt{Pe_r/8.2}\ d_p \tag{4.2-18}$$

$$\text{Length} = 2d_p/Pe_x \tag{4.2-19}$$

Denote the total length of the reactor by L, and the radius by R_t. Then the number of stages in axial and radial directions will be

$$N = L\,Pe_x/2d_p \tag{4.2-20}$$

$$M = R_t\sqrt{8.2/Pe}_r\,/d_p \tag{4.2-21}$$

For the interparticle field, we consider a single, first order, reversible, exothermic reaction which is absolutely controlled by the surface reaction rate step. Also the particle surface temperature is assumed equal to the fluid temperature. So that

$$r_c(c,T) = R_o(1-c)e^{E_1(1-1/T)} - R_o ce^{E_{02}-E_2/T} \tag{4.2-22}$$

c denotes the extent of reaction, R_o is the reaction rate when the extent of reaction is zero and the dimensionless temperature unity. Let

$$Da_I = LR_o/V \tag{4.2-23}$$

then

$$R_{i,j} = \frac{Da_I}{N}\left[(1-C_{ij})e^{E_1(1-1/T_{ij})} - c_{ij}e^{E_{02}-E_2/T_{ij}}\right] \tag{4.2-24}$$

Since the heat released from the particle is equal to the reaction rate multiplied by the change of enthalpy due to the reaction

$$P'_{i,j} = \lambda R_{i,j} \tag{4.2-25}$$

$$\lambda = \Delta H/(\rho C_p T'_o) \tag{4.2-26}$$

Now we can evaluate the temperature and the concentration distributions throughout the fixed bed reactor for a set of given conditions by the following procedures:

1. Calculate N and M by equations (4.2-20) and (4.2-21) for given reactor length and radius as well as Peclet numbers.
2. Take φ and ψ of the first row as the input concentration and temperature.
3. Estimate a reaction rate, R.
4. Compute c and T of the i,j stage by

   $c = \varphi + R$

   $T = \psi + R$
5. Substitute c and T into equation (4.2-24) to obtain the reaction rate, R.
6. If the difference between the calculated and estimated values of R is less than a tolerable error then go to next step, otherwise, go back to step 3.
7. Similarly, calculate the concentration and temperature of other stages in the same row, except the stage at the wall.
8. For the wall stage, compute Stanton number by equation (4.2-15).
9. Estimate a reaction rate and evaluate c and T by

   $c = \varphi + R$

   $T = \psi + \lambda R + Q_i N_{st}$

   where Q_i is given.
10. Substitute c and T into equation (4.2-24)

11. If the difference between the calculated and estimated R is less than a tolerable error, then go on to the next step, otherwise go back to step 9.
12. Compute φ and ψ by equations (4.2-6) and (4.2-9).
13. Repeat the same routine as in the first row, and so on until the last row.
14. The yield will be the average concentration in the last row.

3. Optimal Heat Flux Profile: A Computational Strategy

In Chapter II, the pseudo-optimum search method was applied to find the optimal temperature profile in a one-dimensional reactor, even though we did not specifically mention the method itself. The procedure is:

1. Estimate a temperature profile.
2. Evaluate the concentration and corresponding pseudo-optimum profile by

$$T^*(c) = \frac{E_2 - E_1}{E_{02} - E_1 - \mathrm{Ln}\left(\frac{1-c}{c}\frac{E_1}{E_2}\right)} \qquad (4.3\text{-}1)$$

3. Use this profile as a new estimate of temperature to repeat the cycle until no change can be made.

However, there is some difficulty involved when applying this method to a two-dimensional model; consider the fixed model bed to be divided into N axial sections and M radial arrays. Also suppose that the initial conditions

are fixed. Then for a given heat flux profile the concentration and temperature throughout the reactor can be evaluated. Similar to the one-dimensional case, we can also calculate the optimal temperature corresponding to the local concentration in each of NxM stages. However, it is impossible to assign all of the NxM stage temperatures to the pseudo-optimum values, because not all are independent variables. For this system there are only N independent variables. There can only be N sections of heat flux or N wall stage temperatures, which can be controlled by adjusting the heat flux (so that the heat flux is no longer independent).

An alternative way to apply the pseudo-optimum method is given as follows:

1. For an estimated heat flux profile evaluate the concentration and the temperature in each of NxM stages. Also find the optimal temperature in each stage and denote it by $T^*(C_{ij})$.
2. If there is a disturbance of the wall stage temperature, $T_{k,M}$, then this disturbance, denoted by D_k, will also effect other stage temperatures down stream. The response can be expressed by the following set of difference approximations

$$\Delta T_{ij} = \Delta\Psi_{i-1,j} + \lambda \frac{dR}{dT} \Delta T_{ij} \qquad (4.3\text{-}2)$$

for all i and j, with the boundary conditions:

$\Delta T_{oj} = 0$

$\Delta T_{iM} = 0$ for $i \neq k$

$\Delta T_{kM} = D_k$

where $\psi_{i-1,j}$ is given by equation (4.2-9)

Because $\frac{dR}{dT}$ is a complicated function of temperature and concentration, the response will be a non-linear function of D_k. However, $\frac{dR}{dT}$ is quite small (0.004) in comparison with unity. A rough estimation of the response can be made by assuming $\frac{dR}{dT}$ to be a constant, denoting it by R'. Then

$$\Delta T_{ij} = \frac{\Delta\psi_{i-1,j}}{1-\lambda R'} \text{ , for all i and j} \qquad (4.3\text{-}3)$$

Therefore, the disturbance response in each stage can be expressed roughly by a linear function of the disturbance and is proportional to D_k, and a function of its location. Let this function be

$$f^k_{i,j} \cdot D_k \qquad (4.3\text{-}4)$$

Because the pseudo-optimum temperature in the (i,j) stage is $T^*(C_{ij})$, the best change for this stage is to increase the stage temperature by $T^*(C_{ij}) - T_{ij}$. However, this is not the problem of a single stage but of all the N x M stages. Therefore, we make the objective function give as

$$\sum_{i=1}^{N} \sum_{j=1}^{M} [f^k_{ij} D_k - T^*(C_{ij}) + T_{ij}]^2 \nu_{ij} \qquad (4.3\text{-}5)$$

minimum, where ν_{ij} is the volume of (i,j) stage. This can be done by forcing the differential with respect to D_k to zero. Denoting this solution by D_k^*, gives

$$D_k^* = \frac{\sum_{i=1}^{N}\sum_{j=1}^{M} f_{ij}^k [T^*(C_{ij}) - T_{ij}]\nu_{ij}}{\sum_{i=1}^{N}\sum_{j=1}^{M} (f_{ij}^k)^2 \nu_{ij}} \qquad (4.3\text{-}6)$$

By geometric arguments, we have

$$f_{ij}^k = f_{i-1,j}^{k-1} \text{ for } i = 1, \ldots, k-1 \qquad (4.3\text{-}7)$$

so that

$$f_{i,j}^k = f_{i-k+1,j} \text{ for } k = 1, \ldots, i \qquad (4.3\text{-}8)$$

3. The new setting for the wall stage temperature is

$$T_{k,M|new} = T_{k,M|old} + \frac{\sigma D_k^*}{\sqrt{\sum_{k=1}^{N} (D_k^*)^2/N}} \text{ for } k = 1, \ldots, N \qquad (4.3\text{-}9)$$

where σ is a constant adjusted to control the step size. Since it is not realistic to control the wall stage temperature, the corresponding heat flux, Q, can be obtained by solving

$$T_{k,M} = \psi_{k-1,M} + Q_k N_{st} + \lambda R(C_{kM}, T_{kM}) \qquad (4.3\text{-}10)$$

where N_{st} is Stanton number given by equation (4.2-15).

4. Return to step 1 and iterate the cycle until each D_k^* is smaller than a tolerable error.

4. Results of Computation

Now we must choose some numerical values for parameters, such as input conditions, kinetic constants and size of reactor so that the heat flux profile will be the only variables. In order to compare with the result obtained by Gray, the same data he used are presented here for the computation. The data are given in Table 5.

TABLE 5

PARAMETER VALUES FOR COMPUTATION

Dimensionless input temperature (based on 620°K)	1.0762	
Dimensionless input concentration	0.0382	
Axial length, L	4.524	ft.
Radius, R_t	0.3	ft.
Particle diameter, d_p	0.03	ft.
Mass Peclet number, Pe	11.0	
Thermal Peclet number, Pe'	8.45	
Damkohler number, Da_I	0.2262	
$Da_{III}/Da_I = \Delta H/(\rho C_p T_o)$	2.0	
Kinetic constants, E_1	19.35	
E_{02}	40.35	
E_2	41.35	

As Levenspiel and Bischoff [L6] pointed out, one disadvantage of the finite stage model is that the magnitudes of mass and heat dispersion must be taken to be equal.

However, at uniform radial flow rate the only problem it raises is that the concentration gradient across the section is due to the various reaction rates because of different temperature distributions. In other words, it is the heat dispersion that determines both concentration and temperature gradients. Therefore, we divide the packed bed reactor into radial arrays according to the thermal Peclet number. For a fully developed turbulent flow the axial Peclet number is 2 [K2, M1]. By equations (4.2-20) and (4.2-21), we obtain

$$M = 9.5$$

$$N = 448$$

However, 9.5 x 448 stages are too numerous for the computer currently used to handle. Instead, 4.5 x 112 stages are used to simulate the tubular reactor. Figure 23 shows the comparison of two different simulations by the radial temperature profiles of both cases at z=1 and z=0.5. Figure 24 gives the radial concentration profiles at z=1 and z=0.5. Where z is the dimensionless axial distance.

The algorithm for solving the optimal heat flux profile consists of five programs (see appendix).

1. Procedure Stage evaluates the conversion of a reversible reaction in a single stage and the difference between the local temperature and its pseudo-optimum value. There are three types of stages, i.e. (1) stage which is not at the wall, (2) half stage at the wall, (3) full stage at the wall. Because the second and third types of stages possess different characteristics, this will result in

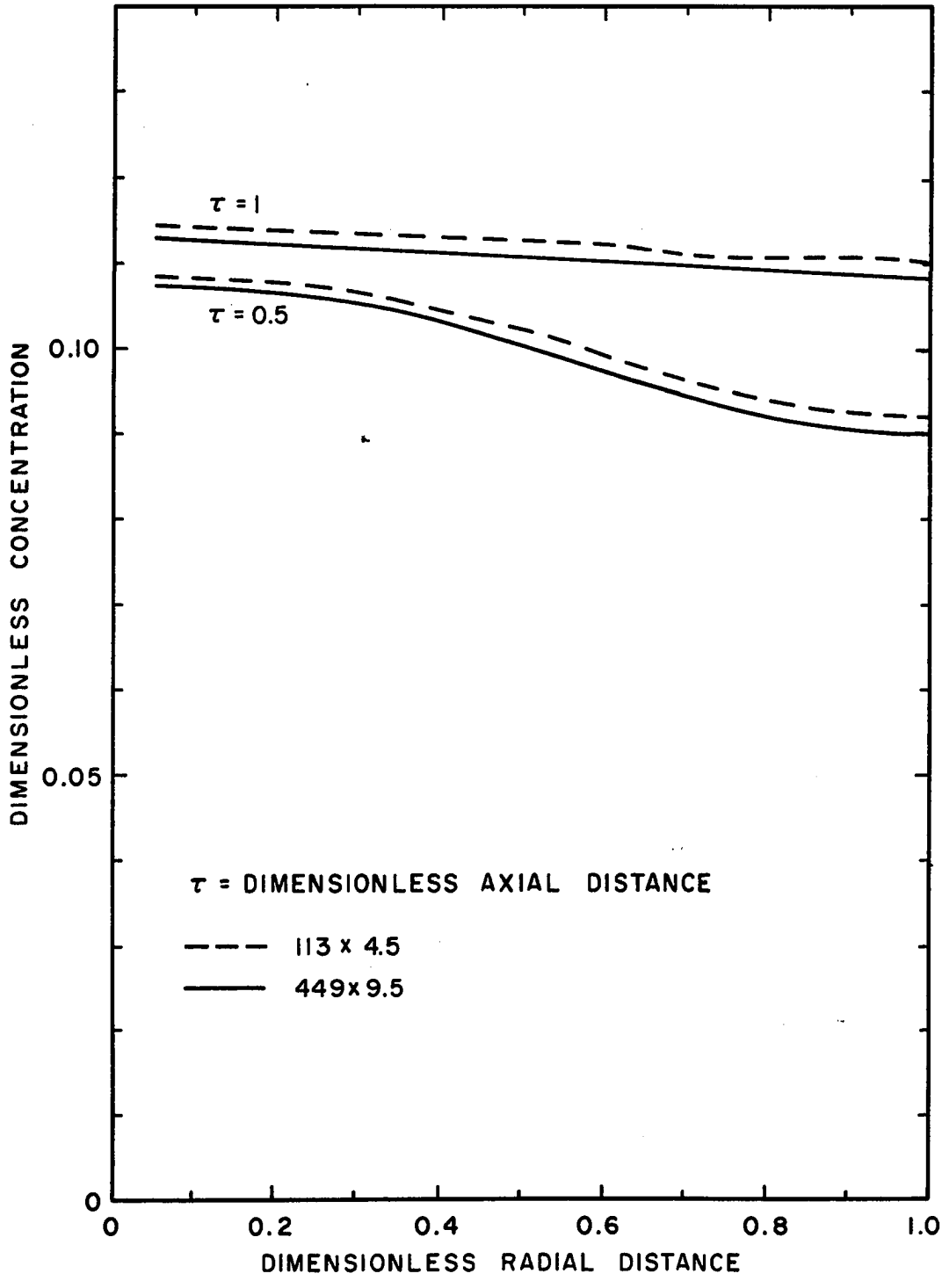


Figure 23.--Comparison of Concentration Calculated Using Different Grid Sizes for Two-Dimensional Reactor Model

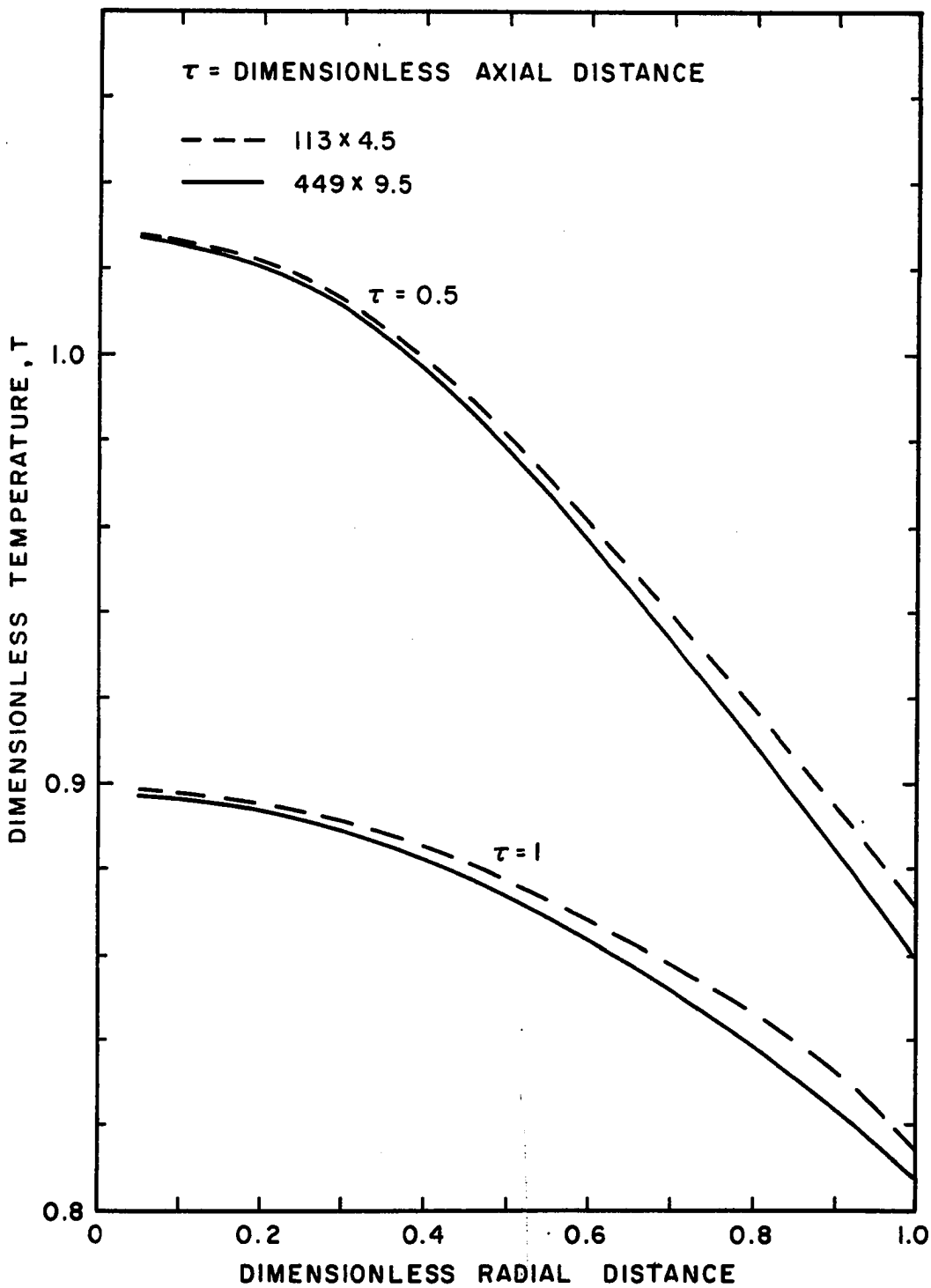


Figure 24.--Comparison of Temperature Calculated Using Different Grid Sizes for Two-Dimensional Reactor Model

an uneven heat flux profile. To avoid this, only the temperature in a half stage at the wall will be adjusted directly. Then the heat flux at this half stage can be evaluated and the same value is adopted for the heat flux in the next full stage at the wall. The flow chart is shown in Figure 25.

2. Procedure Row will compute φ and ψ by equations (4.2-6) and (4.2-9) and execute a row of 'Stage.'
3. Procedure Yield calculates the temperature and concentration distribution throughout the reactor as well as the yield by executing a sequence of 'Row.'
4. Procedure Ascent makes adjustment on the wall stage temperatures by equation (4.3-9). The value of σ is given initially, then the program halves the value in each iteration.
5. The main program combines the function of Yield and Ascent, and iterates the loop until the difference between the yields computed by two consecutive trials is less than 0.0002.

The two sets of heat flux profile were used as the initial estimate for obtaining the optimum. They were plotted in Figure 28 as curve A_o and B_o. The curve A_o was evaluated to give optimal temperature distribution while M = 1. The curve B_o will give uniform temperature when the dimensionless temperature is unity and M = 1. Denote the two series of ascents starting from A_o and B_o as A and B, and their corresponding final results as A_f and B_f. The initial value of

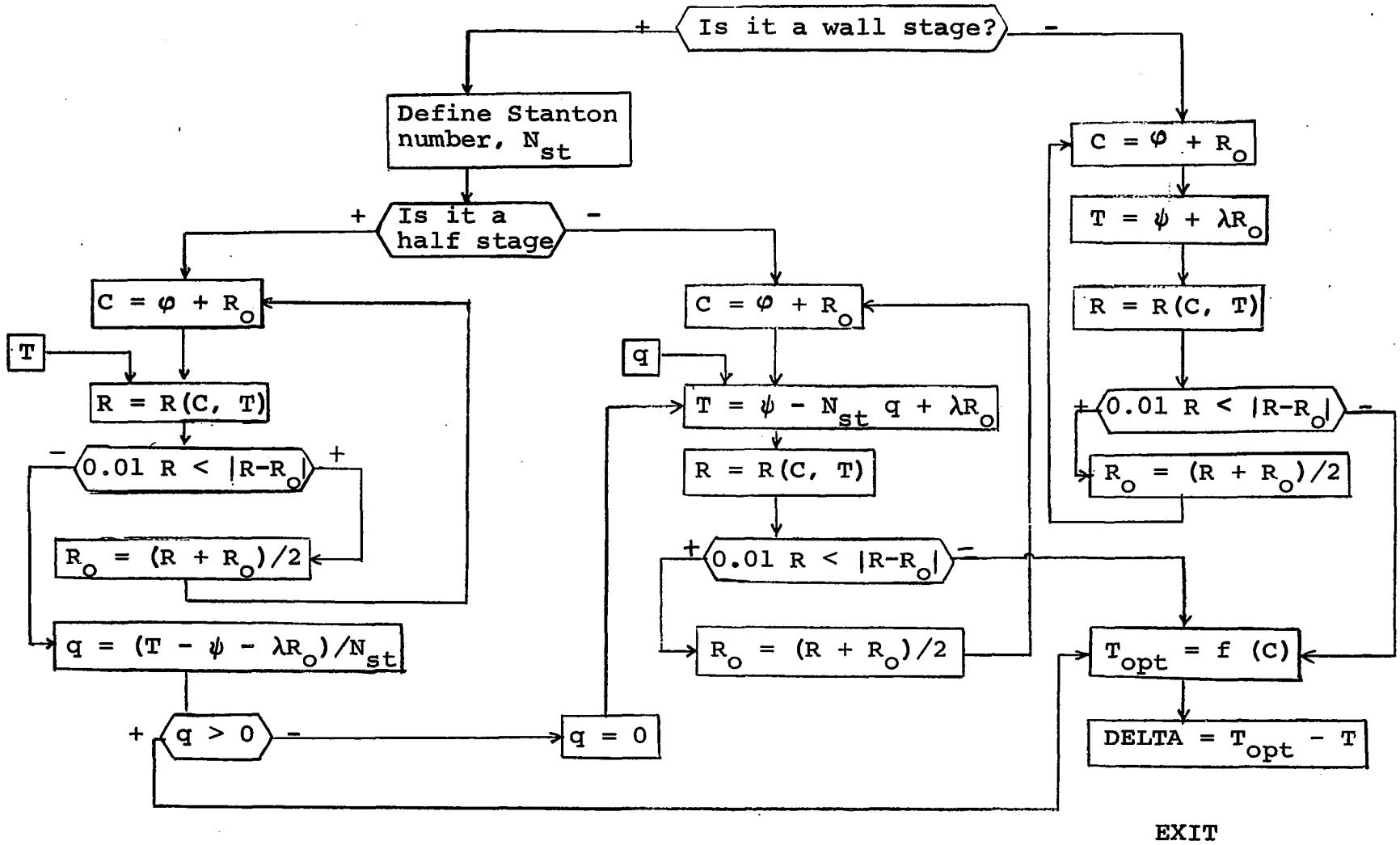


Figure 25.--Flow Chart of Computational Procedure of a Single Stage in Two-Dimensional Reactor Model

σ was given to be 0.08 for series A and 0.04 for series B.

Figure 26 and Figure 27 show the average radial temperature along the reactor of A and B ascending series, respectively. The state trajectories of A_o, A_f, B_o and B_f were given in Table 6 and Table 7. Also the average radial temperature, concentration along the reactor and the heat flux profiles of A_o, B_o, A_f and B_f were plotted in Figure 28, Figure 29 and Figure 30, respectively. Figure 31 and Figure 32 show the values of D* calculated by equation (4.3-9) for A and B series of ascents. The yields of A and B series were plotted in Figure 33. Figure 33 shows that the final yield is 0.1592, compared with a yield of 0.15062 obtained by Gray. However, the difference might be caused by using different mathematical models. Another study was made to adopt Gray's method to our mathematical model. Starting from condition B_o, the yield of consecutive trials were plotted in Figure 33. Denote this series of ascents by C. Even though the final yeild of 0.15734 is quite close to the maximum yield of 0.1592 obtained by pseudo-optimum method, the necessary condition for an optimum is far from being satisfied; at the optimum condition the partial derivative of object function with respect to each control element should be zero, but in this case this isn't true. The actual values of the C ascending series are shown in Figure 34. The radial temperature profiles at various axial distances of A_f and C_f were given in Figure 35 for comparison.

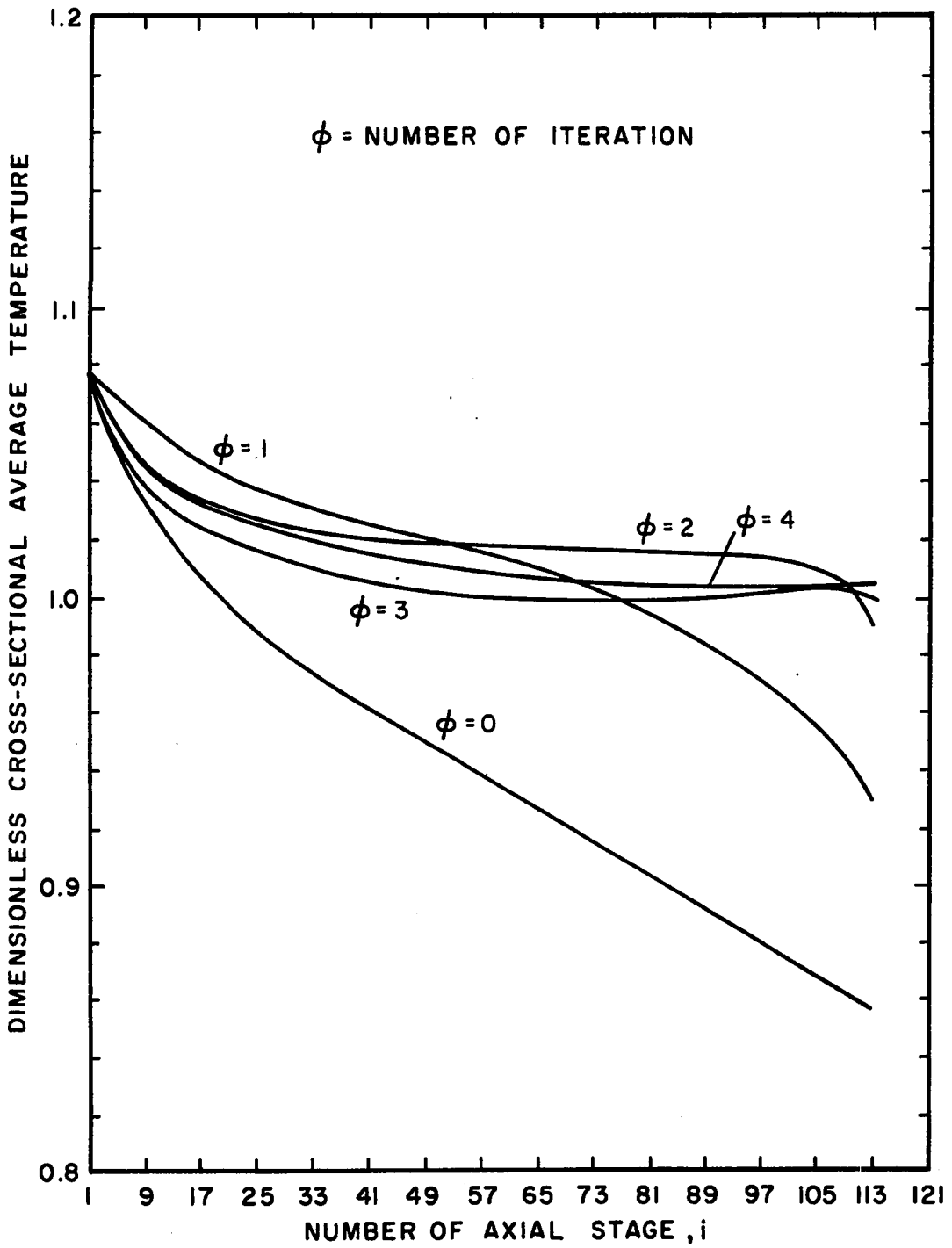


Figure 26.--Cross-Sectional Average Temperature Profiles. Consecutive Trials: Ascending Series-A

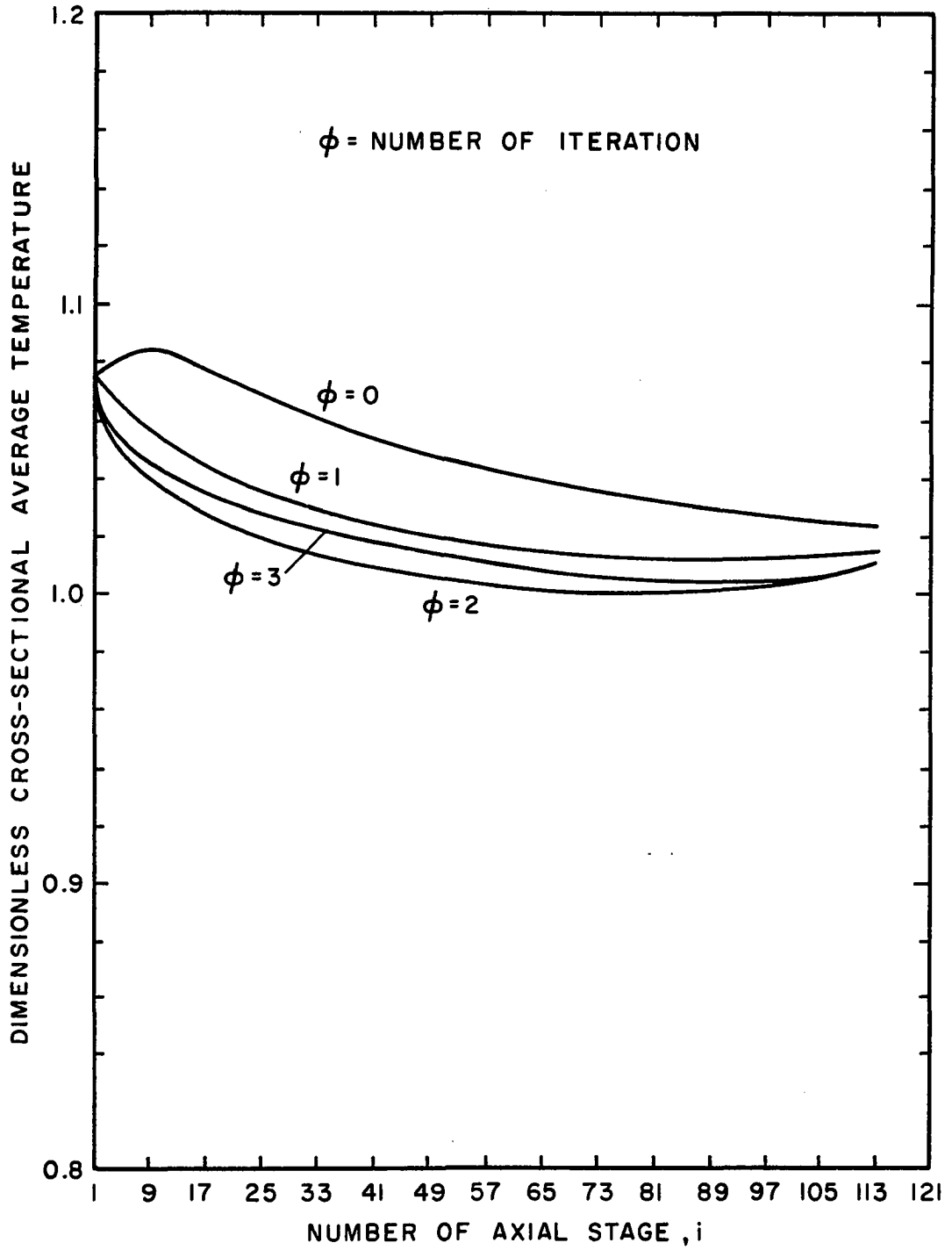


Figure 27.--Cross-Sectional Average Temperature Profiles. Consecutive Trials: Ascending Series-B

TABLE 6

INITIAL AND FINAL CONDITIONS OF FIRST ASCENT SERIES

Dimensionless Distance	Heat Flux, Q	Average Temp.	Average Conc.	D_k^*
0.0	1.362#	1.0762	0.0382	0.14677
	2.02*	1.0762	0.0382	-0.00589
0.0715	0.812	1.0342	0.054342	0.20896
	0.546	1.0433	0.054488	-0.00394
0.143	0.580	1.0071	0.064117	0.25179
	0.432	1.0336	0.066120	-0.00434
0.2145	0.465	0.98836	0.0727722	0.27975
	0.378	1.0263	0.076655	-0.00394
0.286	0.395	0.97367	0.80352	0.30042
	0.340	1.0205	0.086395	-0.00333
0.3575	0.347	0.96110	0.087059	0.31636
	0.310	1.0157	0.095483	-0.00266
0.429	0.311	0.94954	0.092843	0.32839
	0.285	1.0118	0.10402	-0.00203
0.5	0.2835	0.93836	0.09773	0.33662
	0.263	1.0086	0.11210	-0.00204
0.5715	0.261	0.92714	0.10174	0.34076
	0.243	1.0061	0.11977	-0.00190
0.643	0.243	0.991568	0.10492	0.34022
	0.2235	1.0043	0.12709	-0.00110
0.7145	0.227	0.90393	0.10737	0.33417
	0.2045	1.0031	0.13410	-0.00088
0.786	0.214	0.89197	0.10921	0.34141
	0.185	1.1128	0.14082	-0.00083
0.8575	0.202	0.87993	0.11058	0.29970
	0.164	1.0035	0.14728	-0.00089
0.929	0.1923	0.86791	0.11157	0.26240
	0.141	1.0054	0.15344	-0.00057
1.0	0.1833	0.85602	0.11230	0.18113
	0.106	1.0076	0.15924	-0.00329

#Initial condition

*Final condition

TABLE 7

INITIAL AND FINAL CONDITIONS OF SECOND ASCENT SERIES

Dimensionless Distance	Heat Flux, Q	Average Temp.	Average Conc.	D_k^*
0.0	0.382*	1.0762	0.0382	-0.12248
	2.10 #	1.0762	0.0382	0.00137
0.0715	0.365	1.0837	0.055313	-0.12637
	0.542	1.0419	0.054311	0.00105
0.143	0.344	1.0757	0.063899	-0.11962
	0.434	1.0244	0.076420	0.00107
0.2145	0.3238	1.0676	0.071655	-0.11709
	0.387	1.0319	0.65918	0.00096
0.286	0.3043	1.0604	0.79158	-0.10214
	0.338	1.0187	0.086144	0.00079
0.3575	0.2863	1.0541	0.086451	-0.09376
	0.3065	1.0142	0.095237	0.00064
0.429	0.2703	1.0485	0.093533	-0.08560
	0.2815	1.0105	0.10379	0.00050
0.500	0.255	1.0435	0.10039	-0.07760
	0.260	1.0076	0.11190	0.00039
0.5175	0.240	1.0393	0.10702	-0.06965
	0.240	1.0053	0.11959	0.00032
0.643	0.2263	1.0355	0.11341	-0.06153
	0.223	1.0037	0.12694	0.00026
0.7145	0.213	1.0322	0.11955	-0.05309
	0.204	1.0027	0.13396	0.00022
0.786	0.201	1.0293	0.12546	-0.04411
	0.186	1.0024	0.14070	0.00019
0.8575	0.189	1.0268	0.13113	-0.03427
	0.165	1.0030	0.14717	0.00012
0.929	0.1782	1.0247	0.13656	-0.02274
	0.1382	1.0047	0.15336	0.00002
1.0	0.1682	1.0228	0.14177	-0.00534
	0.0633	1.0097	0.15919	-0.00034

*Initial condition

#Final condition

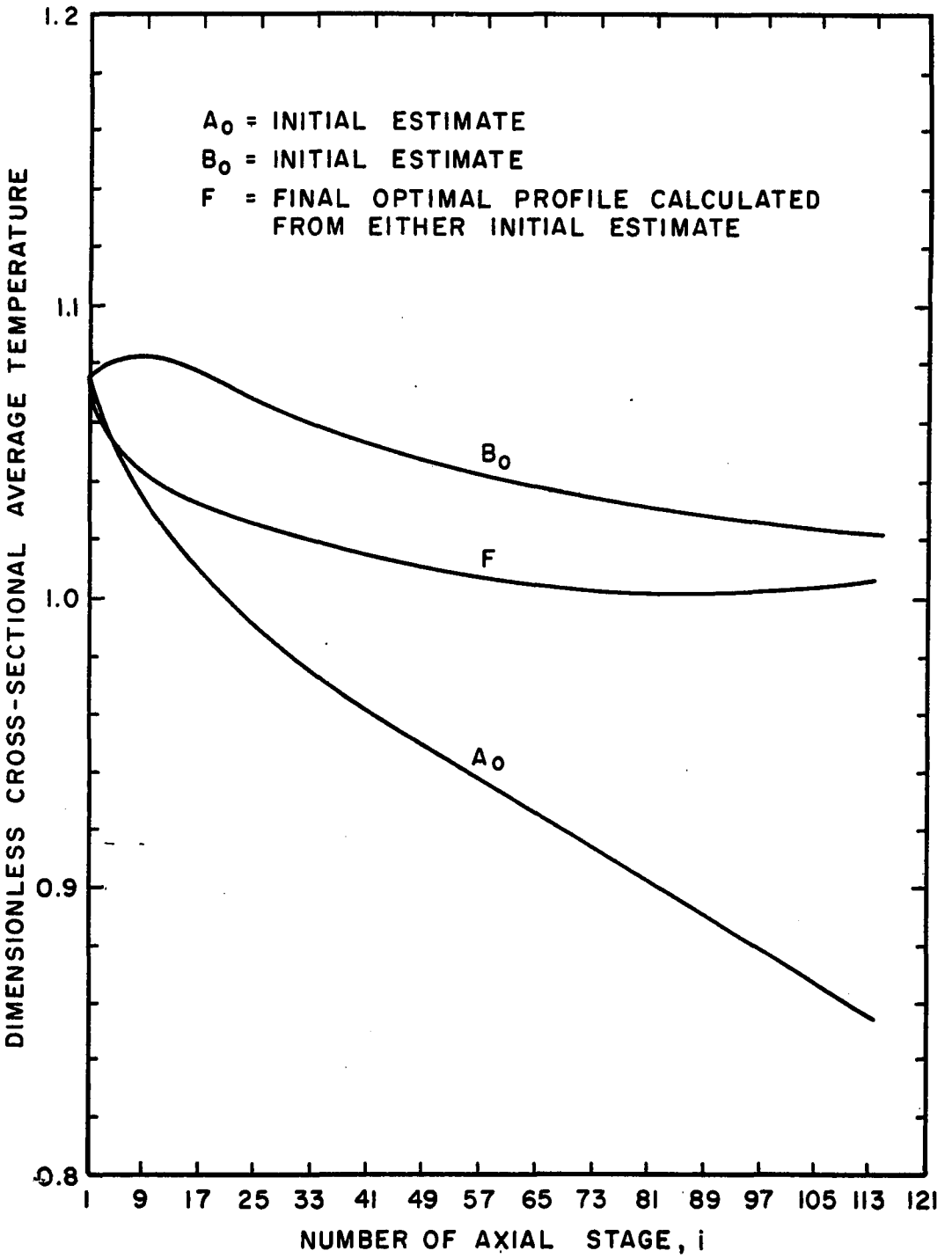


Figure 28.--Initial and Optimal Temperature Profiles For Two-Dimensional Reactor Model

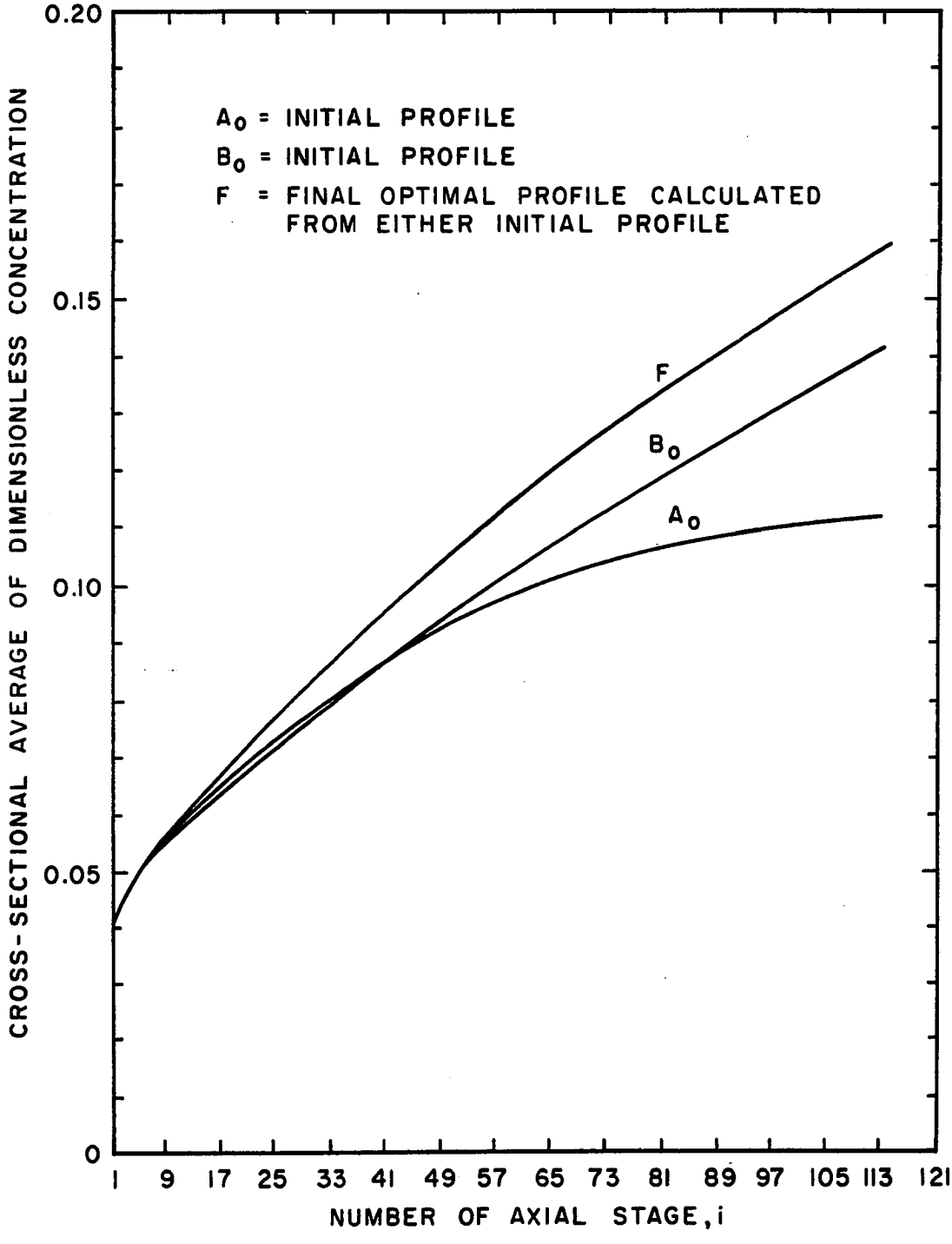


Figure 29.--Initial and Optimal Concentration Profiles For Two-Dimensional Reactor Model

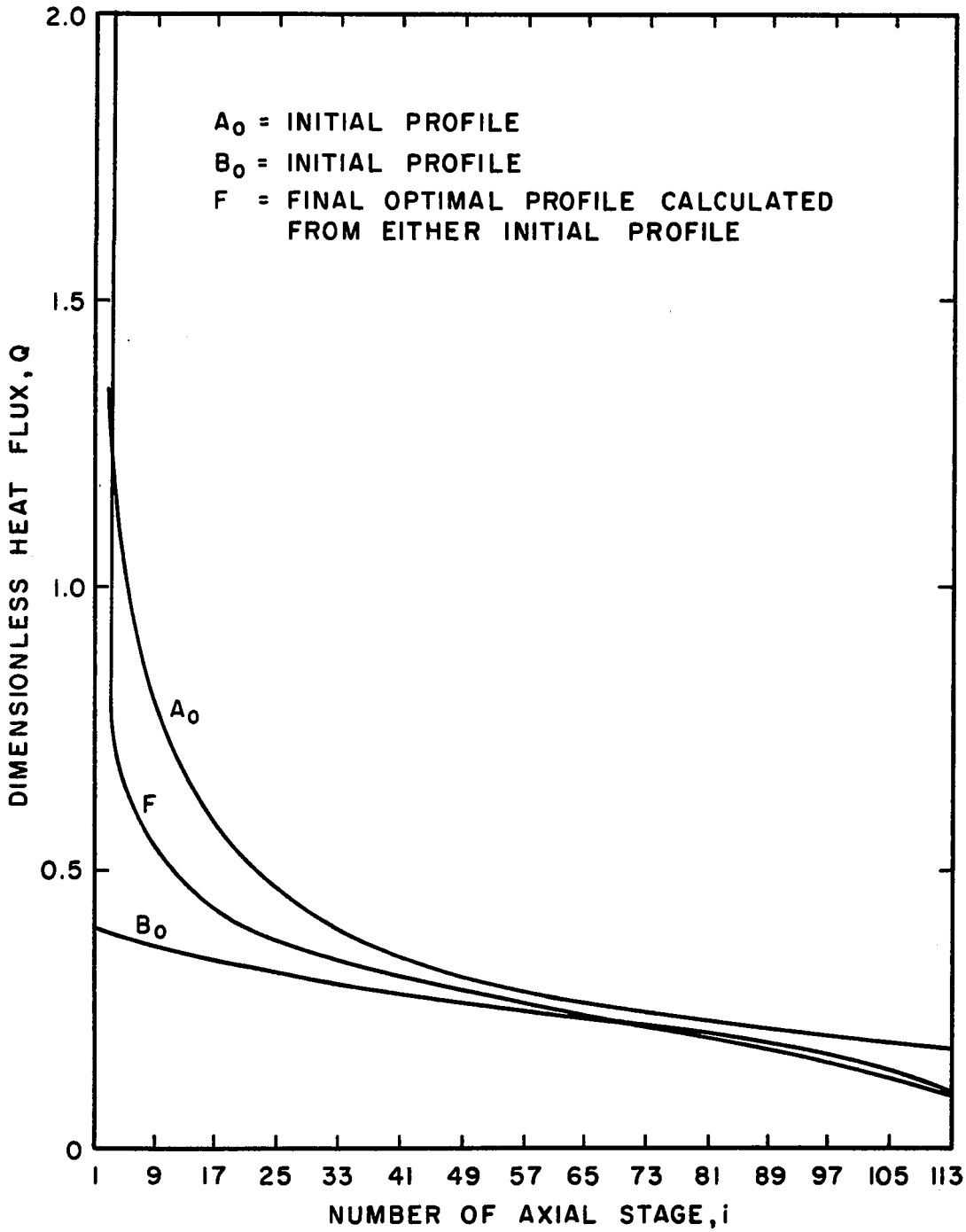


Figure 30.--Initial and Optimal Heat Flux Profiles For Two-Dimensional Reactor Model

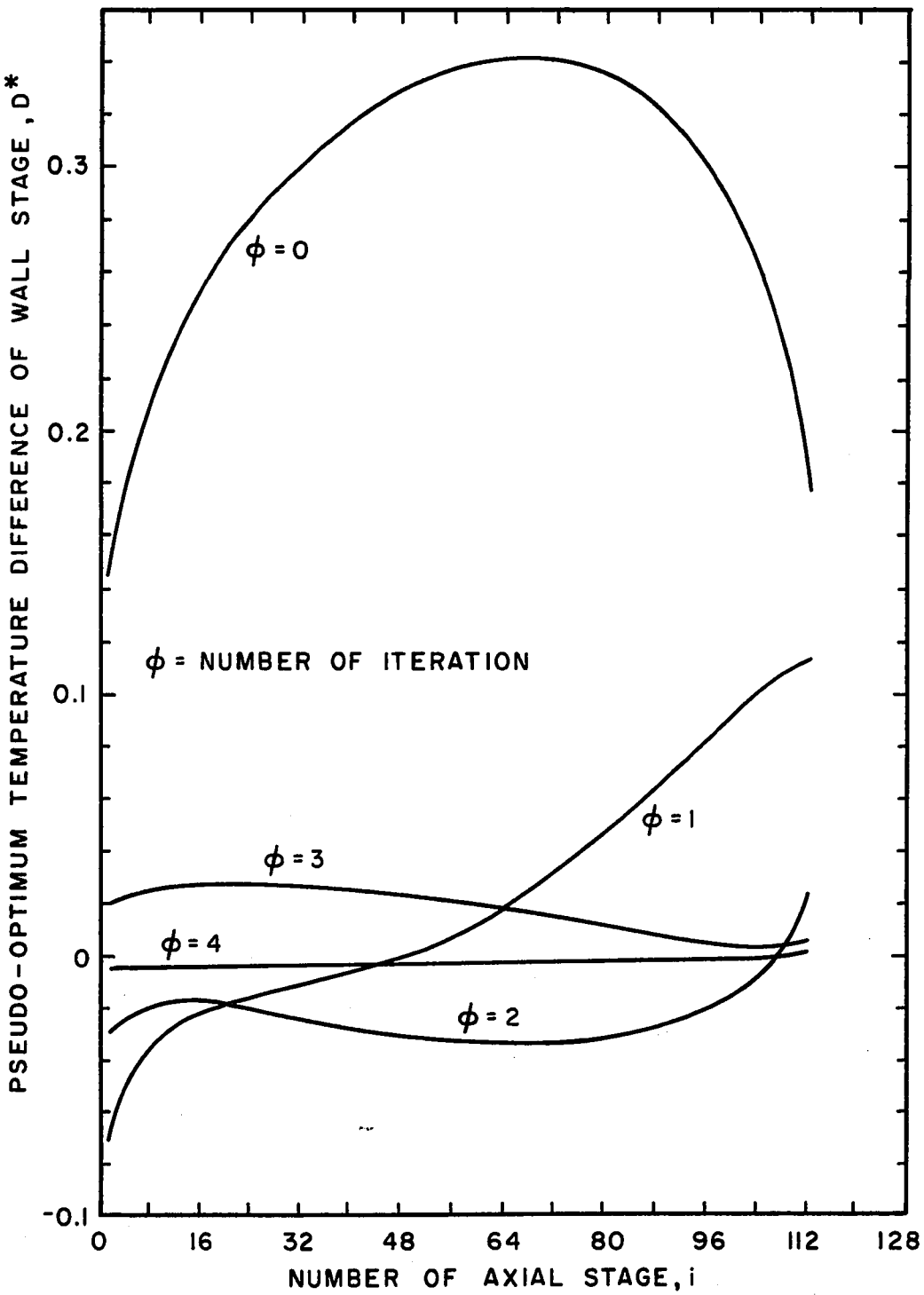


Figure 31.--Pseudo-Optimum Temperature Difference of Wall Stage. Consecutive Trials: Ascending Series-A

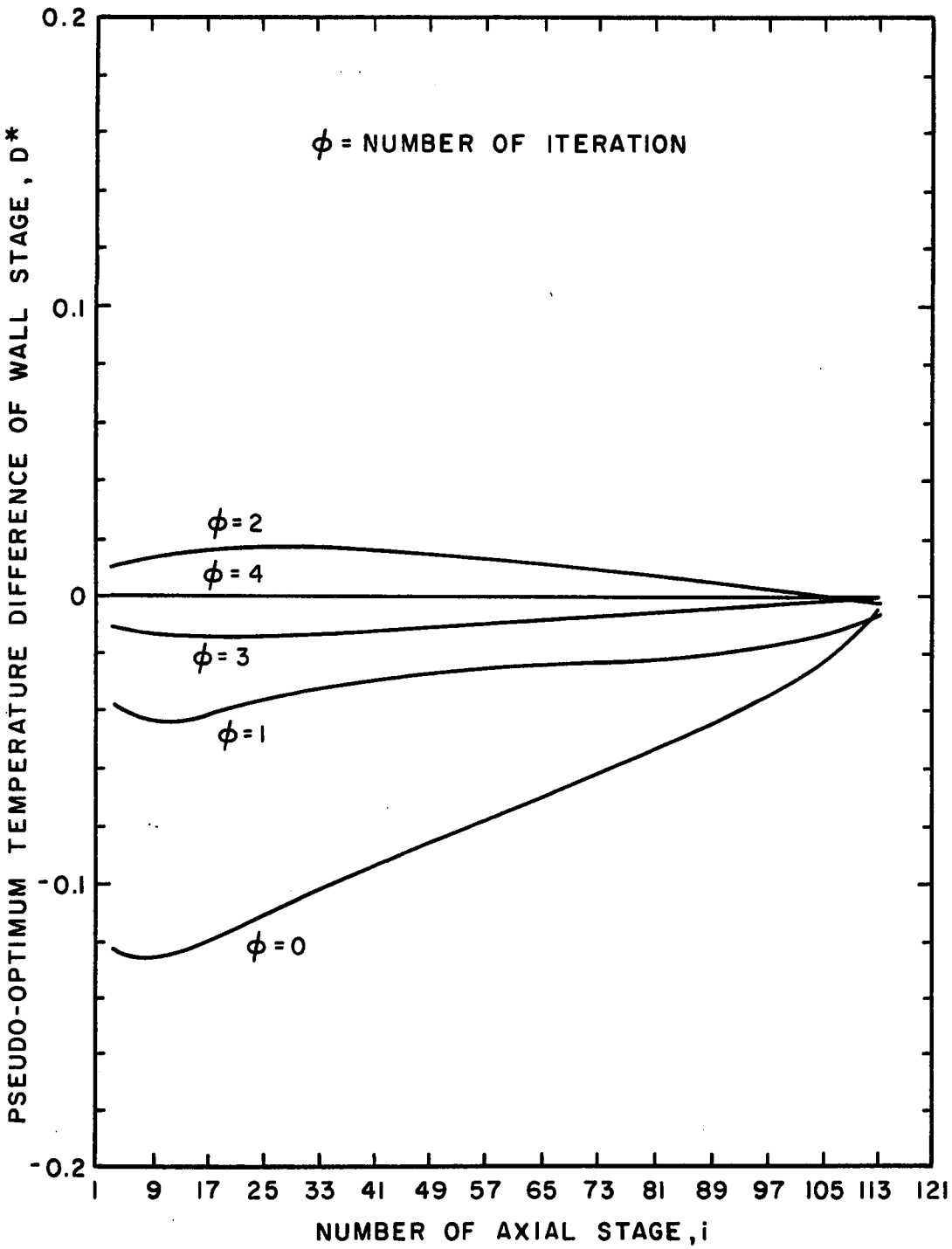


Figure 32.--Pseudo-Optimum Temperature Difference of Wall Stage. Consecutive Trials: Ascending Series-B

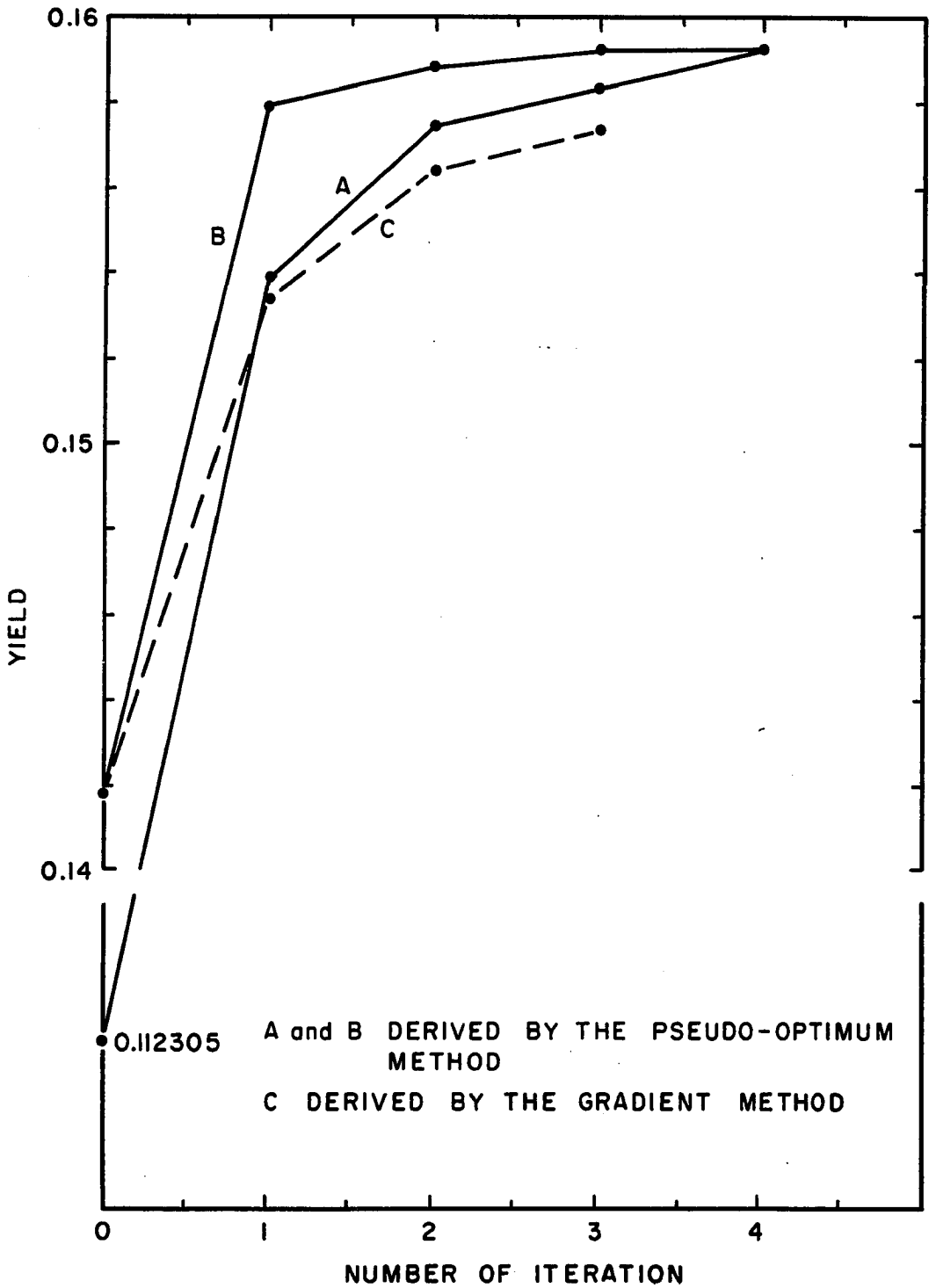


Figure 33.--Comparison of the Yields of Three Ascending Convergence Series. Two-Dimensional Reactor Model

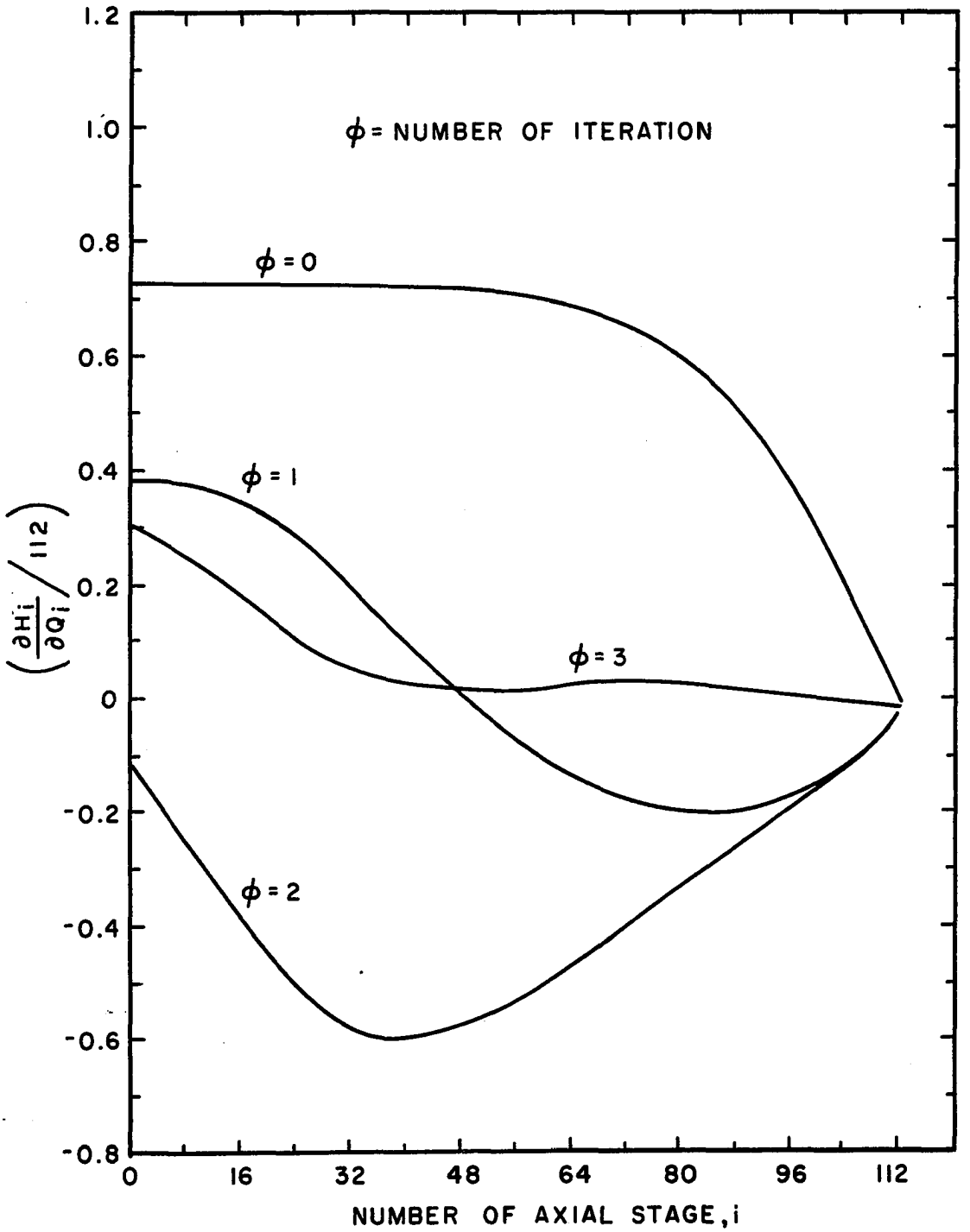


Figure 34.--Gradient in Functional Space of Two-Dimensional Reactor Model. Consecutive Trial: Ascending Series-C

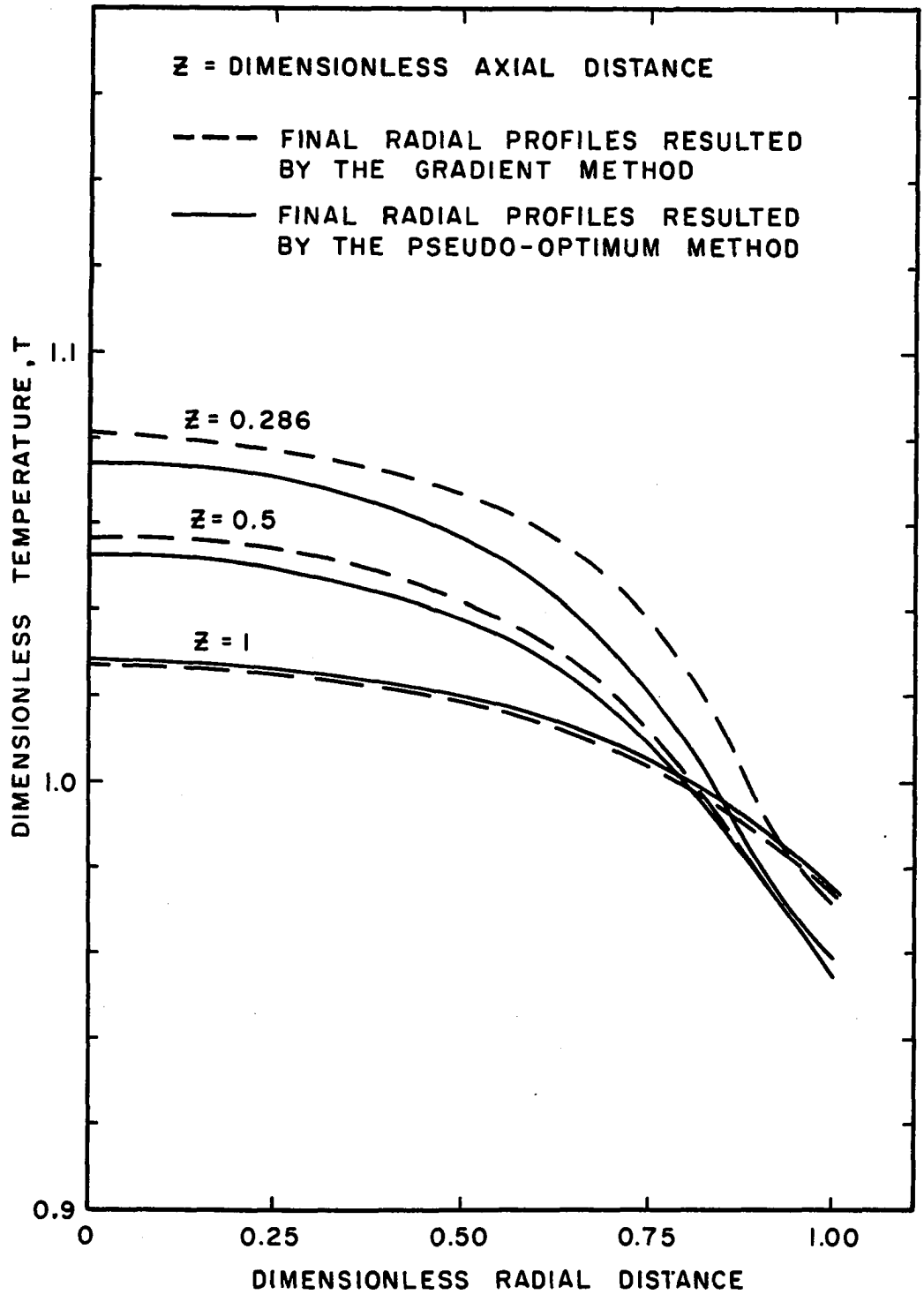


Figure 35.--Comparison of Final Temperature Distributions Calculated by the Pseudo-Optimum Method and the Gradient Method

CHAPTER V

CONCLUSION AND RECOMMENDATION FOR FURTHER WORK

The pseudo-optimum method was successfully applied to solving for the optimal operating conditions of a specific two-dimensional reactor problem. The success of this method is limited to the particular model chosen but there does not seem to be any hindrance to applying the technique to other problems. It should be noted that convergence can not be proven for non-linear problems but only shown by computation. The extension to more generalized problems is discussed as follows:

1. The two-dimensional finite stage model was used to simulate a fixed bed reactor. However, by using other dispersion models, it is still necessary to divide the whole reactor into finite grids for incremental integration. Therefore, the pseudo-optimum temperature can be computed in each grid. Then a similar technique can be used to find the optimal policy.

2. In the problem studied, the catalyst particle temperature was assumed equal to the fluid temperature. However, this is not a necessary assumption. Consider the reaction rate to be

$$\text{Rate} = k_1 (T_s) [(1 - c_s) - c_s/K(T_s)] \qquad (5.2\text{-}1)$$

where c_s and T_s are the surface concentration and temperature. Let the mass transfer coefficient and heat transfer coefficient in the film to be k_p and h_p. At steady state, the surface reaction rate should be equal to the transfer rate from the surface to the fluid, then

$$\text{Rate} = k_p (c_s - c) \tag{5.2-2}$$

$$\text{Rate } \Delta H = h_p (T_s - T) \tag{5.2-3}$$

where c_s and T_s can be represented in terms of fluid concentration and temperature, as

$$c_s = c + \text{Rate}/k_p \tag{5.2-4}$$

$$T_s = T + \text{Rate } \Delta H/h_p \tag{5.2-5}$$

Substitute c_s into the Rate equation, and solve for the Rate, yields

$$\text{Rate} = \frac{k_1[(1 - c) - c/K]}{1 + k_1 (1 + 1/K)/k_p} \tag{5.2-6}$$

The maximum of Rate occurs at

$$\frac{d\ \text{Rate}}{d\ T_s} = 0$$

Let $k_1 = k_1^o\, e^{E_1 (1 - 1/T_s)}$ and $K = e^{I_S - I_H/T_s}$

If $k_p >> k_1$, then the optimal surface temperature can be solved as

$$T_s^* = \frac{I_H}{I_S - \ln K^*} \tag{5.2-7}$$

where

$$K^* = \frac{c}{1-c} - \frac{I_H}{E_1 k_p} \left[k_1 + \frac{c}{1-c} (k_1 + k_p) \right] \tag{5.2-8}$$

By using the relation of equation (5.2-5), the optimal fluid temperature will be

$$T^* = \frac{I_H}{I_S - \ln K^*} + \frac{\Delta H \cdot \text{Rate}}{h_p} \tag{5.2-9}$$

This is the pseudo-optimum temperature. Other computational strategy is similar to the simple case.

3. Even though we considered only the first order reversible reaction, A B, the optimization problem with a general reversible reaction of the form

$$-\frac{d C_A}{dt} = k_1 (C_A^a C_B^b \ldots C_D^d - C_P^p C_R^r \ldots C_S^s/K)a/n \tag{5.3-1}$$

can be carried out by the same routine. The pseudo-optimum temperature will be

$$T^* = \frac{T_{eq}}{1 + \frac{R T_{eq}}{E_2 - E_1} \ln \frac{E_2}{E_1}} \tag{5.3-2}$$

where T_{eq} is the equilibrium temperature.

4. For two consecutive reactions, two simultaneous reactions, or other complicated reaction schemes in a two-dimensional reaction model, the algorithm will be quite different. Because the pseudo-optimum temperature of those reactions not only depends on the local concentration, but also is a function of the state of other stages. However, the pseudo-optimum temperature on the wall stage can still be obtained by using the one-dimensional search method as illustrated in the first example of Chapter III. The computational procedure is as follows:

1). Estimate a heat flux profile, and evaluate the concentration and temperature throughout the reactor.

2). Keep all other wall stage temperatures as obtained from the last step, but vary one wall stage temperature. Then recalculate the concentration and temperature throughout the reactor. Use the one-dimensional search method to locate the best value for that wall stage temperature which will give the maximum yield or profit. Denote this value as D_k^*.

3). The procedure to find D_k^* will consume considerable computer time. For example, if it takes 3 minutes to evaluate the states of 112 x 4.5 stages for a given set of decisions, and seven trials to locate the approximate optimum by the search method, then it will consume 21 minutes to calculate a single D_k^* value, or 18 hours to obtain all of the 112 points for one iteration. However,

the evaluation of each pseudo-optimum point is independent of each other, i.e., the value of D_k^* is a function of the original estimate, but independent of other D_j^*'s. Therefore, if we calculate only a few D_k^* points, then other points can be obtained by interpolation methods.

4). Once we have all the D_k^*, the new setting for the wall stage temperature will be

$$T_{k,M}|_{New} = T_{k,M}|_{Old} + \frac{\sigma\, D_k^*}{\sqrt{\sum_{k=1}^{N} (D_k^*)^2/N}} \qquad \text{for } k = 1, \ldots, N$$

and the corresponding heat flux can be evaluated.

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NOMENCLATURE

A	=	contact wall surface (4.2-13)*
$\bar{\bar{A}}$	=	a matrix (3.3-9)
A_1, A_2	=	proportional constants (3.2-1)
a_1, a_2, a_3	=	concentrations of component A in first, second and third stage respectively (3.2-2)
a'	=	constant of phase equilibrium relation (3.3-2)
b_1, b_2, b_3	=	concentrations of component B in first, second and third stage respectively (3.2-2)
b'	=	constant of phase equilibrium relation (3.3-2)
C	=	concentration of product, mole/liter (2.1-1)
C_{in}	=	sum of concentrations of reactant and product at input (2.1-2)
c	=	extent of reaction or dimensionless concentration, C/C_{in} (2.1-2)
C_p	=	heat capacity (4.1-6)
c_s	=	dimensionless concentration at particle surface (5.2-2)
$\bar{\bar{D}}$	=	matrix (3.3-10)
$\bar{D}$	=	adjoint vector (1.4-3)
D_s	=	element of adjoint vector (1.4-3)
D_c	=	adjoint of c (2.2-1)

*The numbers in parentheses at the end of the definitions refer to the equation number where the symbol was defined or first used.

D_T = adjoint of T (2.2-2)

D_x = adjoint of x (2.2-18)

D_y = adjoint of y (2.2-19)

D_Q = gradient with respect of Q (2.2-8)

D_k = change of wall stage temperature, $\Delta T_{k.M}$ (4.3-2)

D_k^* = optimal value of D_k (4.3-6)

D_z = axial diffusivity (2.1-1)

D_{aI} = first Damkohlor number (2.1-13), (4.1-5)

D_{aIII} = third Damkohlor number (4.1-6)

d = a variable proportional to the liquid flow rate (3.3-4)

d_p = particle diameter (4.2-14)

E_1, E_2, E_{02} = constants (2.1-13)

$\bar{E}$ = vector (3.3-10)

e = constant (3.3-4)

$\bar{\bar{F}}$ = transformation matrix (1.4-2)

$\bar{F}$ = forward vector transformation function (1.1-2)

$\bar{F}'$ = backward vector transformation function

f_s = scale function (1.1-1)

f_i = objective function (1.2-3)

$f_{i,j}$ = a geometric factor (4.3-4)

g = abbreviation of left-hand side of equation (4.1-9)

G = vapor flow rate (3.3-1)

$\bar{G}$ = a vector (1.4-2)

ΔH = enthalpy change per unit reaction (4.1-6)

H = Hamiltonian (1.3-2)

H' = vapor hold-up in each equilibrium plate (3.3-1)

h = liquid hold-up in each equilibrium plate (3.3-1)

h_p = heat transfer coefficient in the film (5.2-3)

h_T = heat transfer coefficient at wall (4.1-8)

i = number of axial stage (4.1-8)

$\bar{\bar{I}}$ = unit matrix (3.3-13)

j = number of radial stage

K = reaction equilibrium constant (5.2-1)

K^* = equilibrium constant at optimal temperature (5.2-8)

k_1, k_2 = reaction constants (2.2-7)

k_p = mass transfer coefficient in the film (5.2-2)

L = length of reactor (2.1-3)

L' = liquid flow rate (3.3-1)

M = total number of radial increments (4.2-21)

N = total number of axial stage (2.1-3)

N_{st} = Stanton number (4.2-15)

Pe = Peclet number (4.1-2)

P' = change of temperature due to chemical reaction (4.2-7)

P = total perturbation (1.4-11)

q = decision variable (1.1-1)

q = heat flux (2.1-7)

Q = dimensionless heat flux (2.1-7)

Q' = flow rate (4.2-12)

R = dimensionless reaction rate (2.1-4)

Rt = radius of reactor

r, r_c = chemical reaction rate (2.1-1)

R' = initial range of one-dimensional search (3.2-13)

S = total number of state variables (1.1-1)

S' = temperature change due to heat flux at wall stage (4.2-1)

s = ratio of length to radius (4.1-2)

s = integral variable (3.3-11)

s = number of state variable (1.1-1)

T = dimensionless temperature (2.1-6)

T_o' = the absolute temperature, of which the dimensionless temperature is based upon (4.2-26)

T_{in} = input dimensionless temperature (4.1-7)

T_L = lower limit of T (3.2-2)

T_U = upper limit of T (3.2-2)

T_{opt} = optimal temperature (2.1-14)

T^* = pseudo-optimum temperature (3.2-8)

t = time

u = flow velocity (2.1-1)

V = flow velocity

$\bar{X}$ = state vector (1.1-2)

x = a component of state vector (1.1-1)

x = liquid concentration (3.3-1)

Y = total profit (1.3-8)

y = net profit of a single stage (1.2-4)

y = vapor concentration (3.3-1)

Z = distance (2.1-1)

z = dimensionless distance (1.1-1)

z = a component of Green's vector (1.3-3)

Greek Letters

γ = a constant (3.2-2)

λ = ratio of temperature increase to reaction (2.1-6)

η = maximum percentage conversion (2.1-11)

μ = LaGrange multiplier (1.4-12)

θ = terminal time (1.1-1)

θ = residence time (3.2-3)

ν = volume of stage (4.2-3)

σ = a constant adjusted to control the step size (4.3-9)

ξ = ratio of fluid volume to total volume (4.2-3)

ρ = density of fluid (4.1-6)

Δ = a constant adjusted to control the step size (3.1-9)

Superscript

$=$ = matrix

$-$ = column matrix or vector

T = transpose of matrix

APPENDIX

COMPUTER PROGRAMS

In this appendix the listing of computer programs is given to present detailed computational procedures. Explanation and purpose of the programs are given in comments or in self-explained labels. All programs were written in Osage Algol and the rules of this language are given in a publication by R. B. Worrell: The Osage Algorithmic Language-Osage Algol, Norman, Oklahoma, 1964. A few specific symbols are illustrated as follows:

Δ	and
∇	or
:=	replace
¬	not
$	integer divide
|	left or right of absolute value
Begin...End	bracket
SLON(2)	If sense light 2 ON
McProcedure	Subroutine

```
Program 210;
Comment search the maximum conversion for one dimensional reactor;
Begin Integer i, k, l, N, code, section;
Real DELTA, DP, C0, T0, lambda, M1, E1, E2, E01, E02, DA1, K0,
     LENGTH;
McProcedure One D(211, 1, 16);
McProcedure Adjoint (212, 1, 7);
READPT (N, C0, T0, DP, DELTA, lambda, E1, E2, E01, E02, DA1,
        code);
Begin Real Array Q, Q1, WF[0:N], DQ[0:N+1],YLD [0:30];
Real Array DRDC, DRDT[0:N];
Format F4(J1, 'Q[', I3,']', S4, R5),
       F2(J1, 5(S2, R5));
If SLON(5) Then Begin READPT(Q[2], Q[N]);
For i:=2 Step 1 Until N Do
Q[i]:=Q[2]+(Q[N]-Q[2])/(N-2)*(i-2);
End Else READPT(For i:=2 Step 1 Until N Do Q[i]);
section:=1;
If SLON(6) Then READPT(For i:=1 Step 1 Until (N-1)$section+ Do
  WF[i]) Else For i:=1 Step 1 Until (N-1)$section +1 Do WF[i]:=1.;
K0:=DA1/(N-1);
l:=1;
For i:=2 Step 1 Until N Do PRINT(F4, i, Q[i]);
L1: One D(YLD[1], N, code, C0, T0, Q, lambda, E1, E2,
          E01, E02, K0, DRDC, DRDT);
If YLD[1-1] < YLD[1]Then Else Goto EXIT;
```

```
For i:=2 Step 1 Until N Do Q1[i]:=Q[i];
l:=l+1;
L2: Adjoint (DRDC, DRDT, lambda, 2, N, code, DP, DQ);
For i:=2 Step 1 Until N Do Q[i]:=Q1[i]-DQ[i];
Goto L1;
EXIT: If SLON(4) Then Begin
DP:=DP/2.; Goto L2; End;
End End of Program;

Program 211;
Comment the contration and temperature profile in one dimensional
        reactor;
Procedure One D(yld, N, code, C0, T0, Q, lambda, E1, E2, E01,
                E02, K0, DRDC, DRDT);
Value Q, lambda, E1, E2, E01, E02, K0, C0, T0;
Integer N, code;
Real yld, C0, T0, lambda, E1, E2, E01, E02, K0;
Real Array Q, DRDC, DRDT;
Begin Integer i, j;
Real Rate;
Boolean SECOND, Tfix;
Real Array C, T, flux, DTDQ[0:N];
Format D2(J7, 'SECOND DERIVATIVES:'),
DD(J2, 'STAGE', I3, 10(J2, 5(S2, R5)));
Switch OPTION:=P1, P2, P2, P3, P3, P3;
Format F13(J7, 'TOTAL CONVERSION', S3, R5),
```

```
        F10(J1, 'STAGE NO.',  S4, 'CONCENTRATION', S2, 'TEMPERATURE',
        S4, 'HEAT FLUX', S6, 'DCDQ'),
        F12(J2, S3, I3, S5, 4(R6, S3));
McProcedure Stage (202, 1, 30);
C[1] :=C0
T[1] :=T0;
Goto OPTION[code];
P1: For i:=1 Step 1 Until N Do flux[i]:=Q[i];
    SECOND:= False;
    T fix:= False;
    Goto P5;
P2:
P3: For i:=2 Step 1 Until N Do T[i]:=Q[i];
    SECOND:=False;
    T fix:=True;
    Goto P5;
P5: For i:=2 Step 1 Until N Do
Stage(i, code, C[i-1], T[i-1], C[i], T[i], Rate, lambda,
      E1, E2, E01, E02, K0, True, Tfix, flux[i], -1.,
      DRDC[i], DRDT[i]);
yld:=C[N];
PRINT(F13, yld);
PRINT(F10);
For i:=1 Step 1 Until N Do
PRINT(F12, i-1, C[i], T[i], flux[i]);
End;
End of Procedure;
```

```
Program 212;
Procedure Adjoint (DRDC, DRDT, lambda, I0, N, code, DP, ADJT);
Real Array DRDC, DRDT, ADJT;
Real lambda, DP;
Integer N, code, I0;
Begin
Integer i;
Real ADJC, SUM;
Switch OPTION:=L1, L2, L3, L4;
Format FI(J7, 'ADJOINT OF TEMP', 300(J2, 4(S2, R5))), FH(J2,
       6(S2, R5));
ADJC:=1.;
ADJT[N+1]:=0;
Goto OPTION code ;
L1: For i:=N Step -1 Until I0 Do Begin
ADJT[i]:=ADJT[i+1]+DRDT[i]*ADJC+lambda*DRDT[i]*ADJT[i+1];
ADJC:=ADJC+DRDC[i]*ADJC+lambda*DRDC[i]*ADJT[i+1];
If SLON(1) Then PRINT(FH, DRDC[i], DRDT[i], ADJC, ADJT[i]);
End; Goto L5;
L2: For i:=N Step -1 Until I0 Do Begin
ADJC:=ADJC*(1.+DRDC[i]);
ADJT[i]:=ADJC*DRDT[i];
If SLON(1) Then PRINT(FH, DRDC[i], DRDT[i], ADJC, ADJT[i]);
End; Goto L5;
L3: For i:=N Step -1 Until I0 Do
ADJT[i]:=DRDT[i];
If SLON(1) Then PRINT(FH, For i:=I0 Step 1 Until N Do ADJT i );
```

```
Goto L5;
L4:
L5:SUM:=0;
For i:=I0 Step 1 Until N Do
SUM:=SUM+ADJT[i]^2;
SUM:=SQRT(SUM); If SLON(3) Then READPT(DP);
For i:=I0 Step 1 Until N Do
ADJT[i]:=ADJT[i]*DP/SUM;
PRINT(FI, For i:=I0 Step 1 Until N Do ADJT[i]);
End of Program;

Program 202;
Comment Conversion of a reversible reaction in a single stage,
        while the first and second derivatives may also be
        evaluated;
Procedure Stage(il, jl)
          Input conc and temp:(XC, XT)
          Output conc and temp:(C, T)
          Reaction rate:(Rate)
          Kinetic constant:(lambda, E1, E2, E01, E02, K0)
          If it is wall stage:(WALL)
          If it controls stage temperature directly:(Tfix)
          The heat flux if it is wall stage:(flux)
          The change of wall stage by change of flux:(DWALTDQ)
          First derivative:(DRDC, DRDT);
Value  Tfix;
Integer il, jl;
```

```
Real XC, XT, C, T, Rate, flux, DWALTDQ, lambda, E1, E2, E01,
     E02, K0;
Boolean WALL, Tfix;
Real DRDC, DRDT;
Begin
Real CA, CB, K1, K2, DR1DT, DR2DT, R1, R2, OPT;
Integer j, r, l, lk;
Format F5(J1, 'STAGE(',I3,I3,')', 6(S1, R6)),
       F6(J1, 6(S1, R6));
If SLON(1) Then PRINT(F6, j1, XT, XC, flux);
r:=0;
REPEAT: If r < 3 Then CB:=XC+Rate Else CB:=(XC+CB+Rate)/2.;
           CA:=1.-CB;
If Tfix Then Goto L3;
If WALL Then T:=XT+DWALTDQ*flux+Rate*lambda
Else T:=XT+Rate*lambda;
L3: K1:=K0*EXP(E01-E1/T);
    K2:=K0*EXP(E02-E2/T);
    R1:=K1*CA;
    R2:=K2*CB;
If SLON(1) Then PRINT(F6, K1, K2, R1, R2, Rate);
    If 0.01*(R1-R2) < |R1-R2-Rate| Then Else Goto RESULT;
    Rate:=R1-R2;
    r:=r+1;
    Comment SLON(7) means no axial diffusion;
    If r < 12 △¬SLON(7) Then Goto REPEAT;
```

```
RESULT: C:=CB;
If T fix Then Begin flux:=(T-XT-Rate*lambda)/DWALTDQ;
If flux < 0 Then Begin flux:=0; Tfix:=False;
     r:=1; Goto REPEAT; End End;
     DRDC:=-(K1+K2);
If SLON(8) Then Begin
OPT:=(E2-E1)/(E02-E01-LN(CA/CB*E1/E2));
DRDT:=OPT-T;
End Else Begin
     DR1DT:=K1*CA*E1/T^2;
     DR2DT:=K2*CB*E2/T^2;
     DRDT:=DR1DT-DR2DT;
End;
If SLON(1) Then PRINT(F5, i1, j1, C, T, Rate, DRDC, DRDT);
End of Program;
```

```
Program 203;
Begin
Comment This is the main program for evaluating the optimal
        temperature distribution in a series of stirred tank
        reactors;
Real UPLMT, RANGE, DELTA, Y, L0, L1, RATIO;
Integer i, j, MU, Nu, N, TRIAL;
Real Array X1, X2, X3, T, T1, OPT, H, H1[0:25], XX1, XX2, XX3
          [0:25];
McProcedure STG(204, 1, 10);
McProcedure YIELD(205, 1, 7);
McProcedure SEARCH(206, 1, 6);
Real Procedure YLDI(I, TT);
Real TT;
Integer I;
Begin
Integer k;
Format FMT(J2, 'YLD=', R5);
Real K1, K, K4, K5;
k:=I;
If 355. < TT Then TT:=355.;
STG(TT,H[k],X1[k-1], X2[k-1], X3[k-1], XX1[k], XX2[k], XX3[k]);
For k:=I+1 Step 1 Until N Do
STG(T[k], H[k], XX1[k-1], XX2[k-1], XX3[k-1], XX1[k], XX2[k],
    XX3[k]);
If SLON(1) Then PRINT(FMT,XX3[N]);
```

```
YLDI:=XX3[N];
End of real procedure;

Real Procedure YLD(I, DELTA);
Integer I;
Real DELTA;
Begin Integer k; Real Y;
Format FMT(J2, 'YLD=', R5);
For k:=1 Step 1 Until N Do
T1[k]:=T k +DELTA*(OPT[k]-T[k]);
YIELD(Y, T1, H, XX1, XX2, XX3, N);
If SLON(1) Then PRINT(FMT, Y);
YLD:=Y;
End of real procedure;

Format
F1(J7, 'STAGE TEMPERATURE PSEUDO-OPTIMUM'),
F2(J2, I3, 2(S2, R5)),
F3(J7, 'CONCENTRATION OF X3', R5, J2, 'TEMPERATURE', S6,
   'INCREMENT', S7, 'X1', S11, 'X2', S11, 'X3'),
F4(J2, 5(S2, R5));
READPT(N, TRIAL, MUM RANGE, RATIO);
READPT(For i:=1 Step 1 Until N Do T[i]);
READPT(For i:=1 Step 1 Until N Do H[i]);
YIELD(Y, T, H, X1, X2, X3, N);
PRINT(F3, Y);
```

```
For i:=1 Step 1 Until N Do
PRINT(F4, T[i], H[i], X1[i], X2[i], X3[i]);
NU:=1;
GO: PRINT(F1);
For i:=1 Step 1 Until N Do Begin
UPLMT:=T[i]+RANGE/2.;
SEARCH(i, UPLMT, RANGE, OPT[i], YLDI, TRIAL);
PRINT(F2, i, T[i], OPT[i]);
End;
If SLON(5) Then SEARCH(0, 1., 1., DELTA, YLD, TRIAL)
   Else DELTA:=1.;
For i:=1 Step 1 Until N Do
T[i]:=T[i]+DELTA*(OPT[i]-T[i]);
YIELD(Y, T, H, X1, X2, X3, N);
PRINT(F3, Y);
For i:=1 Step 1 Until N Do
PRINT(F4, T[i], H[i], X2[i], X2[i], X3[i]);
RANGE:=RANGE*RATIO;
NU:=NU+1;
If NU ≤ MU Then Goto GO;
If SLON(2) Then PUNCH(For i:=1 Step 1 Until N Do T[i],
    For i:=1 Step 1 Until N Do H[i]);
End of program;

Program 204;
Procedure STG(T, H, X01, X02, X03, X1, X2, X3);
```

```
Comment Conversion in a single stirred tank reactor;
Real T, H, X01, X02, X03, X1, X2, X3;
Begin Real K1, K2;
Format F1(J2, 'STAGE', 6(S2, R5));
If T < 335. Then T:=335.;
If 355. < T Then T:=355.;
K1:=5.D10 *EXP(-18000./1.987/T)*H;
K2:=3.33 D17 *EXP(-30000./1.987/T)*H;
X1:=((4.*K1*X01+1.)**.5-1.)/2./K1;
X2:=(X02+K1*X1**2)/(1.+K2);
X3:=X2+0.3*X1-0.3;
If SLON(1) Then PRINT(F1, T, K1, K2, X1, X2, X3);
End of program;

Program 205;
Procedure YIELD(YLD, T, H, X1, X2, X3, N);
Comment To evaluate the yield of a series stirred tank reactors
        for given temperatures and holding time;
Real YLD;
Real Array T, H, X1, X2, X3;
Integer N;
Begin
McProcedure STG(204, 1, 10);
Integer i;
Format F1(J2, 'YIELD PROCEDURE', S2, R5);
X1[0]:=1.;
```

```
X2[0]:=0;
X3[0]:=0;
For i:=1 Step 1 Until N Do
STG(T[i], H[i], X1[i-1], X2[i-1], X3[i-1], X1[i], X2[i], X3[i]);
YLD:=X3[N];
If SLON(1) Then PRINT(F1, YLD);
End of procedure;

Program 206;
Procedure SEARCH(I, UPLMT, RANGE, OPT, YIELD, TRIAL);
Real UPLMT, RANGE, OPT;
Integer I, TRIAL;
Real Procedure YIELD;
Begin
Integer k;
Real L, R, YLDX, YLDOPT, X, tau, DEL, X1;
Format F1(J2, 'SEARCH PROCEDURE', 2(S2, R5));
tau:=1.618033989;
L:=UPLMT-RANGE;
R:=UPLMT;
k:=1;
OPT:=X:=L+RANGE/tau;
YLDOPT:=YIELD(I, X);
k:=k+1;
X:=L+RANGE/tau^2;
A01: YLDX:=YIELD(I, X);
DEL:=RANGE/tau^k+1;
```

```
If YLDX < YLDOPT Then Else Goto A20;
A10: If X < OPT Then Else Goto A12;
     X1:=R-DEL;
     Goto B10;
A12:R:=X
     X1:=L+DEL;
     Goto B10;
A20:If X < OPT Then Else Goto A22;
A21:R:=OPT;
     X1:=L+DEL;
     Goto A23;
A22:L:=OPT;
     X1:=R-DEL;
A23:OPT:=X;
     YLDOPT:=YLDX;
B10:If k ≤ TRIAL ∆ OPT < 355. ∆ 335.< OPT  Then Else Goto EXIT;
X:=X1;
k:=k+1;
Goto A01;
EXIT:If SLON(1) Then PRINT(F1, OPT, YLDOPT);
If 355. < OPT Then OPT:=355.;
If OPT < 335. Then OPT:=335.;
End of Procedure;
```

```
Program 210;
Begin
Comment This is the main program for evaluating the discrete
        optimal flow rate of a 6 tray absorption column;
Real UPLMT, RANGE, RATIO, XO, XN1, dfinal, DELTA;
Real LOW, tau, e;
Integer i, j, MU, N, TRIAL, NSTEP, LENGTH, NU, M;
Real Array X, XJO, XDESIR[1:6], XX1, XX2[1:6, 0:10],J, J2[0:10],
           d, dopt, d2[0:10], PHISTEP, PSISTEP[1:48, 1:6];
Integer Array H[1:10];
McProcedure SECTION (213, 1, 17);
McProcedure PERFORM (212, 1, 17);
McProcedure SEARCH (211, 1, 7);
Format F1 (J2, 'STAGE ESTIMATION PSEUDO-OPTIMUM'),
       F2 (J2, I3, 2(S3, R5));

Real Procedure YLD (I, Z);
Real Z;
Integer I;
Begin Integer k;
Format FMT (J2, 6(S2, R5));
If 0<I Then Else Goto C2;
C1: Comment evaluate the value of J, when there is a
    distrubance at I stage;
If Z<LOW Then Z:=LOW;
For k:=1 Step 1 Until N Do X[k] := XX1[k, I-1];
```

```
k:=I;
SECTION (k, H[k], Z, e, tau, N, M, XO, XN1, X, XDESIR, J[k-1],
        J2[k], PHISTEP, PSISTEP, True, True);
For k:=I+1 Step 1 Until NSTEP+1 Do
SECTION (k, H[k], d[k], e, tau, N, M, XO, XN1, X, XDESIR, J2[k-1],
        J2[k], PHISTEP, PSISTEP, False, True);
Goto C3;
C2: Comment evaluate the value of J when the estimated profile
    move toward its pseudo optimum profile;
For k:=1 Step 1 Until NSTEP Do
d2[k]:=d[k]+Z*(dopt[k]-d[k]);
PERFORM (NSTEP, H, d2, e, tau, N, M, XO, XN1, XX2, XJ0, XDESIR,
        J2, dfinal, PSISTEP, True);
C3: If SLON (2) Then PRINT (FMT, J2[NSTEP+1]);
Comment because SEARCH will searches the largest value,
        but we need the minimum value of J2, so that;
YLD:=-J2[NSTEP+1];
End of real procedure;

READPT (LOW, dfinal, X0, XN1, e, tau,
        N, M, NSTEP, LENGTH, TRIAL, MU, RANGE, RATIO);
READPT (For i:=1 Step 1 Until N Do XJ0[i],
        For i:=1 Step 1 Until N Do XDESIR[i],
        For i:=1 Step 1 Until NSTEP Do d[i],
        For i:=1 Step 1 Until NSTEP Do H[i]);
j:=0;
```

```
For i:=1 Step 1 Until NSTEP Do
j:=j+H[i] ;
If j<LENGTH Then H[NSTEP+1]:= LENGTH-j Else H[NSTEP+1] :=1;
PERFORM (NSTEP, H, d, e, tau, N, M, X0, XN1, XX1, XJ0, XDESIR,
         J, DFINAL, PHISTEP, PSISTEP, False);
NU:=1;
CO: PRINT (F1);
For i:=1 Step 1 Until NSTEP Do Begin
UPLMT:=d[i]+RANGE/2.;
SEARCH (i, UPLMT, RANGE, LOW, dopt i , YLD, TRIAL);
PRINT (F2, i, d[i], dopt[i]);
End;
If SLON (6) Then
SEARCH (0,1.,1.,0,DELTA,YLD,TRIAL) Else DELTA:=1.;
For i:=1 Step 1 Until NSTEP Do
d[i]:=d[i]+DELTA*(dopt[i]-d[i]);
PERFORM (NSTEP, H, d, e, tau, N, M, X0, XN1, XJ0,XDESIR, J,
         dfinal, PHISTEP, PSISTEP, False);
RANGE:=RANGE*RATIO;
NU:=NU+1;
If NU MU Then Goto CO;
End of program;


Program 211;
Procedure SEARCH (I, UPLMT, RANGE, LOW, OPT, YIELD, TRIAL);
Real UPLMT, RANGE, LOW, OPT;
```

```
Begin
Integer k;
Real L, R, YLDX, YLDOPT, X, tau, DEL, X1;
Format F1 (J2, 'SEARCH PROCEDURE', 2(S2, R5));
tau:=1.618033989;
L:=UPLMT-RANGE;
R:=UPLMT;
k:=1;
OPT:=X:=L+RANGE/tau;
YLDOPT:=YIELD (I, X);
k:=k+1;
X:=L+RANGE/tau^2;
A01: YLDX:=YIELD (I, X);
DEL:=RANGE/tau^k+1;
If YLDX YLDOPT Then Else Goto A20;
A10: If X OPT Then Else Goto A12;
     L:=X;
     X1:=R-DEL;
Goto B10;
A12:R:=X;
    X1:=L+DEL;
    Goto B10;
A20: If X OPT Then Else Goto A22;
A21: R:=OPT;
     X1:=L+DEL;
     Goto A23;
```

```
A22: L:=OPT:
     X1:=R-DEL;
A23: OPT:=X;
     YLDOPT:=YLDX;
B10: If k≤TRIAL ∧ LOW<OPT  Then Else Goto EXIT;
X:=X1;
k:=K+1;
Goto A01;
EXIT: If SLON (1) Then PRINT (F1, OPT, YLDOPT);
If OPT<LOW Then OPT:=LOW;
End of procedure;

Program 212;
Procedure PERFORM (NSTEP, H, d, e, tau, N, M, X0, XN1,
          XX, XJ0, XDESIR, J, dfinal, PHISTEP, PSISTEP, TRY);
Real Array d, XX, XJ0, XDESIR, J, PHISTEP, PSISTEP;
Integer Array H;
Integer NSTEP, N, M;
Real e, tau, X0, XN1, dfinal;
Boolean TRY:
Begin
Format F1 (J7, S7, 'D', S11, 'X1', S11, 'X2', S11, 'X3', S11,
       'X4', S11, 'X5', S11, 'X6',), F2 (J3, ' J= ', R5);
McProcedure SECTION (213, 1, 21);
Integer i, j;
Real Array X 1:N ;
```

```
If ¬TRY Then PRINT(F1);
J[0]:=0;
For i:=1 Step 1 Until N Do
X[i]:=XX[i,0]:=XJ0[i];
D[NSTEP+1]:=dfinal;
For i:=1 Step 1 Until NSTEP+1 Do Begin
SECTION (i, H i, d i, e, tau, N, M, X0, XN1, X, XDESIR, J[i-1],
         J[i],PHISTEP, PSISTEP, True, TRY);
If ¬TRY Then For j:=1 Step 1 Until N Do XX[j,i]:=X[j];
End;
PRINT (F2, J[NSTEP+1]);
End of procedure;

Program 213;
Procedure SECTION (ISTEP, H, d, e, tau, N, M, X0, XN1, X,
          XDESIR, J1, J2, PHISTEP, PSISTEP, NEW, TRY);
Real Array X, XDESIR, PHISTEP, PSISTEP;
Integer ISTEP, H, N, M;
Real d, e, tau, J1, J2, X0, XN1;
Boolean NEW, TRY;
Begin
McProcedure MATEXP (214, 1, 6);
McProcedure MATMPY (215, 1, 6);
Real Array A, PHI, PSI[1:N,1:N], D, Y2[1:N,1:2], MM[1:2],
           Y1, Y3[1:N];
Integer i, j, h;
```

```
Real DIFF, f, g;
Format F1(J2,8(S2, R5));
If SLON(1) Then PRINT(F1, H, d, e, tau, J1, J2);
Comment define matrix A, D, and MM;
For i:=1 Step 1 Until N Do
For j:=1,2 Do D[i,j]:=0;
D[1,1]:=d/e;
D[N,2]:=1./e;
MM[1]:=X0;
MM[2]:=XN1;
If NEW Then Else Goto OLD;
f:=-(d=1.)/e;
g:=d/e;
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do A[i,j]:=0;
For i:=1 Step 1 Until N Do A[i,i]:=f;
For i:=2 Step 1 Until N Do Begin
A[i,i-1]:=g; A[i-1,i]:=1./e;  End;

Comment evaluate the matrix PHI and PSI;
MATEXP (A, PHI, PSI, N, M, tau);
If ¬TRY Then For i:=1 Step 1 Until N Do
        For j:=1 Step 1 Until N Do Begin
h:=N*(ISTEP-1)+i;
PHISTEP[h,j]:=PHI[i,j];
PSISTEP[h,j]:=PSI[i,j];
```

```
End;  Goto L0;
OLD: Comment if PHI and PSI are given;
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do Begin
j:=N*(ISTEP-1)-i;
PHI[i,j]:=PHISTEP[h,j];
PSI[i,j]:=PSISTEP[j,j];
End;
L0:
J2:=J1;
h:=0;
L1: Comment change of X after tau;
h:=h+1;
DIEF:=0;
MATMPY (PHI, N, N, X, 1, Y1);
MATMPY (PSI, N, N, D, 2, Y2);
MATMPY (Y2, N, 2, MM, 1, Y3);
For i:=1 Step 1 Until N Do
X[i]:=Y1[i]+Y3[i];
If ¬TRY ∇ SLON(1) Then
PRINT (F1, d, For i:=1 Step 1 Until N Do X[i]);
If SLON(5) Then Else Goto L2;
Comment an option on how to evaluate J;
For i:=1 Step 1 Until N Do
DIFF:=DIFF+(X[i]-XDESIR[i])^2;
Goto L3;
```

```
L2: DIFF:=(X[N]-XDESIR[N])^2;
L3: J2:=J2+DIFF;
If h<H Then Goto L1;
End of SECTION:

Program 214;
Procedure MATEXP (A, PHI, PSI, N, M, tau);
Comment PHI is EXP(A*tau) and PSI is the integeral of
        EXP(A*s) ds for s from 0 to tau, where A is a
        square matrix;
Real Array A, PHI, PSI;
Integer N, M;
Real tau;
Begin
Real Array AA, Am 1:N,1:n ;
Integer i, j, m;
Real mfactr, mfactrl;
Format F1(J2,8(S2,R5)), F2(J7,'PROCEDURE MATEXP');
McProcedure MATMPY (215, 1, 6);
McProcedure MATSUM (216, 1, 5);
m:=1;
Comment unit matrix;
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do
PHI[i,j]:=PSI[i,j]:=0;
For i:=1 Step 1 Until N Do Begin
```

```
PHI[i,i]:=1.;
PSI[i,i]:=tau;
End;
m:=2;
mfactr:=1.;
mfactrl:=2.;
MATSUM (PHI, N, N, A, tau);
MATSUM (PSI, N, N, A, tau^2/mfactrl);
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do
AA[i,j]:=A[i,j];
SERIES: m:=m+1;
mfactr:=(m-1)*mfactr;
mfactrl :=m*mfactrl;
MATMPY (A, N, N, AA, N, Am);
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do
AA[i,j]:=Am[i,j];
MATSUM (PHI, N, N, AA, tau^(m-1)/mfactr);
MATSUM (PSI, N, N, AA, tau^m/mfactrl);
If m<M Then Goto SERIES;
If SLON(1) Then Begin
PRINT (F2);
For i:=1 Step 1 Until N Do
PRINT (F1, For j:=1 Step 1 Until N Do PHI[i,j]);
For i:=1 Step 1 Until N Do
```

```
PRINT (F1, For j:=1 Step 1 Until N Do PSI[i,j]);
End;
End of procedure MATEXP;

Program 215;
Procedure MATMPY (A, N, M, B, L, C);
Comment matrix multiplication;
Real Array A, B, C;
Integer N, M, L;
Begin Integer i, j, k;
If 1 L Then Else Goto L1;
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until L Do Begin
C[i,j]:=0;
For k:=1 Step 1 Until M Do
C[i,j]:=C[i,j]+A[i,k]*B[k,j];
End; Goto EXIT;
L1: For i:=1 Step 1 Until N Do Begin
C[i]:=0;
For k:=1 Step 1 Until N Do
C[i]:=C[i]+A[i,k]*B[k];
End;
EXIT: End of MATMPY;

Program 216;
Procedure MATSUM (A, N, M, B, f);
```

```
Comment sum of two matrices;
Real Array A, B;
Integer N, M;
Real f;
Begin Integer i,j;
For i:=1 Step 1 Until N Do
For j:=1 Step 1 Until N Do
A[i,j]:=A[i,j]+f*B[i,j];
End of MATSUM;
```

Sample Data For Absorption Tower Problem

0.68	0.85	0
0.417	1.58	1.
6	10	3
30	6	3
0.34	1.	0.0613266
0.113454	0.15776	0.19542
0.22743	0.25465	0.09199
0.17018	0.2366	0.29313
0.341156	0.3819727	0.85
0.85	0.85	3
3	3	

```
Program 200;
Comment the main program to find an optimal operating condition
        for a two dimensional tubular reactor with a single
        reversible reaction;
Begin
McProcedure Yield(201, 1, 13);
McProcedure Ascent(204, 1, 6);
Integer N, M, i, j, l, m, n;
Real M1, C0, T0, DP, DA1, JJ, K0, SQSUM;
READPT(N, M, M1, C0, T0, DA1, DP);
Begin Real Array DELTA, factor[1:N, 1:M], TW, TWX, factor2,
     flux[1:N$2], YLD[0:20], Area[0:1, 1:M];
Format F1(J2, 6(S2, R5));
READPT( For i:=3 Step 1 Until N_1 Do TW i$2 );
If ¬ SLON(3) Then READPT( For i:=2 Step 1 Until N Do
        For j:=1 Step 1 Until M Do factor[i, j]);

Area[1,1]:=0.25/M1^2;
Area[0,1]:=1./M1^2;
Area[0,M]:=(M1-0.25)/M1^2;
Area[1,M]:=(2.*M1-1.)/M1^2;
For j:=2 Step 1 Until M-1 Do Begin
JJ:=j; Area[0,j]:-(2.*JJ-1.)/M1^2;
JJ:=j-.5;  Area[1,j]:=(2.*JJ-1.)/M1^2;
End;
K0:=DA1/(N-1);
n:=N$2; m:=2;
```

```
L1: For i:=m, m+1 Do Begin
    If i-i$2 *2=0 Then 1:=0 Else 1:=1;
    For j:=1 Step 1 Until M Do SQSUM:=SQSUM + factor[i,j]^2
    *Area[1,j];
    End;
factor2[n]:=SQSUM;
If i < N Then Begin
n:=n-1; m:=m+2;
Goto L1; End;
If SLON(1) Then PRINT(F1, For i:=1 Step 1 Until N$2 Do factor2[i]);
1:=1;
L2: Yield(YLD 1 ,N, M1, M, C0, T0, K0, TW, flux, Area, DELTA);
If 0.0002 < |YLD[1]-YLD[1-1]| Then Else Goto EXIT;
L3: Ascent(DELTA, factor, factor2, Area, TW, N, M, DP);
1:=1+1;
Goto L2;
EXIT: End of program; End;

Program 201;
Comment evaluate the concentration and temperature distributions
        throughout the reactor for a given condition;
Procedure Yield (yld, N, M1, M, C0, T0, K0, TW, flux, Area,
                 DELTA);
Integer N, M;
Real yld, M1, C0, T0, K0;
Real Array TW, flux, Area, DELTA;
```

```
Begin Integer i, j, NEVEN;
Real Array C, T[0:M+1], Rate[1:M];
Format F12(J2, 6(S2, R5)),
       F11(J7, 'INPUT CONCENTRATION', S2, R5, J2, 'INPUT
           TEMPERATURE', S2, R5),
       F13(J3, 'TOTAL CONVERSION', S2, R6);
McProcedure Row(205, 1, 13);

If SLON(1) Then PRINT(F12, N, M1, C0, T0, K0);
For j:=1 Step 1 Until M Do Begin
C[j]:=C0;
T[j]:=T0;
End;
PRINT(F11, C0, T0);
For i:=2 Step 1 Until N Do
Row(i, M, M1, C, T, TW[i$2], flux[i$2], Area, Rate, K0, DELTA);
If N-N$2*2=0 Then NEVEN:=0 Else NEVEN:=1;
yld:=0;
For j:=1 Step 1 Until M Do
yld:=yld+Area[NEVEN, j]*C[j];
PRINT(F13, yld);
End of procedure;


Program 202;
Comment conversion of a reversible reaction in a single stage;
```

```
Procedure Stage(Cin, Tin, C, T, Rate, K0, flux, WALL, HALF,
                M1, DELTA);
Real Cin, Tin, C, T, Rate, K0, flux, M1, DELTA;
Boolean WALL, HALF;
Begin
Real CA, CB, R1, R2, OPT, ST, E1, E2, E01, E02, lambda;
Integer i, j, r;
Boolean Tfix;
Format F6(J1, 8(S1, R5));
If SLON(1) Then PRINT(F6, Cin, Tin, flux, K0, Rate);
Comment some given kinetic constants;
E1:=19.35;
E2:=40.35;
E01:=19.35;
E02:=41.35;
lambda:=2.;
If WALL Then Begin
Comment define the Stanton number;
If HALF Then ST:=-M1*M1/(M1-0.25) Else ST:=-M1*M1/(2.*M1-1.);
Comment if it is a half stage, then the stage temperature is
        controlled directly;
T fix:=HALF;
If SLON(5) Then T fix:=False;
End Else T fix:=False;

Comment evaluate the Rate by iteration method;
```

```
r:=0
REPEAT: If r < 3 Then CB:= Cin+Rate
                 Else CB:=(Cin+CB+Rate)/2.;
CA:=1.-CB;
If T fix Then Goto L3;
If WALL Then T:=Tin+ST*flux+Rate*lambda
        Else T:=Tin+Rate*lambda;
L3: R1:=K0*CA*EXP(E01-E1/T);
    R2:=K0*CB*EXP(E02-E2/T);
If SLON(1) Then PRINT(F6, R1, R2, Rate);
If 0.01*(R1-R2)<|R1-R2-Rate| Then Else Goto RESULT;
Rate:=R1-R2
r:=r+1;
If r < 12 Then Goto REPEAT;
RESULT: C:=CB;
If T fix Then Else Goto L4;
flux:=(T-Tin-Rate*lambda)/ST;
If flux < 0 Then Begin
   flux:=0;
   T fix:=False;
   r:=0;
   Goto REPEAT;
End;
L4:OPT:=(E2-E1)/(E02-E01-LN(CA/CB*E1/E2));
DELTA:=OPT-T;
If SLON(1) Then PRINT(F6, Cin, Tin, C, T, OPT, DELTA);
```

```
If SLON(3) Then PUNCH(T);
End of procedure;

Program 204;
Comment make a new estimation on wall stage temperature based
        on DELTA, which is computed from Yield;
Procedure Asent (DELTA, factor, factor2, Area, TW, N, M, DP);
Real Array DELTA, factor, factor2, Area, TW;
Real DP;
Integer N, M;
Begin Integer i, j, l, EVEN, m;
Real SUM;
Real Array DELTATW[1:N$2+1];
Format F9(J7, 'STAGE', S5, 'DELTA TW', S2, 'WALL STAGE TEMP'),
       F10(J2, I3, 6(S2, R5));

PRINT(F9);
l:=1; m:=2;
L1: DELTATW[l]:=0;
For i:=m Step 1 Until N Do Begin
If i-i$2*2=0 Then EVEN:=0 Else EVEN:=1;
For j:=1 Step 1 Until M Do
DELTATW[l]:=DELTATW[l]+DELTA[i, j]*factor[i-m+2, j]*Area[EVEN,j];
End; DELTATW[l]:=DELTATW[l]/factor2[l];
l:=l+1;
m:=m+2;
```

```
If m ≤ N Then Goto L1;
SUM := 0;
For l:=1 Step 1 Until N$2 Do
SUM:=SUM+DELTATW[l]^2;
SUM:=SQRT(SUM/N*2.);
For l:=1 Step 1 Until N$2 Do Begin
TW[l]:=TW[l]+DELTATW[l]*DP/SUM;
PRINT(F10, l*2, DELTATW[l], TW[l]);
End; DP:=DP/2.;
End of program;

Program 205;
Comment execute a row of stages;
Procedure Row(i, M, M1, C, T, TW, flux, Area, Rate, K0, DELTA);
Integer i, M;
Real M1, TW, flux, K0;
Real Array C, T, Area, DELTA, Rate;
Begin
Integer j, J1, J2, ONE;
Real JJ, Cave, Tave;
Real Array Cin, Tin, Cout, Tout[0:M+1];
Boolean WALL, EVEN, HALF;
Format F12(J2, 'ROW:', I3, S2, 'HEAT FLUX:', R5 'AVE CONC:',
       R5, 'AVE TEMP:', R5),
       F21(J2, 'CONCENTRATION', 6(S2, R5)),
       F22(J2, 'TEMPERATURE', 6(S2, R5)),
```

```
        F23(J2, S7, 6(S2, R5));
McProcedure Stage (202, 1, 13);

EVEN:=i-i$2*2=0;
Tout[M]:=TW;
If EVEN Then ONE:=0 Else ONE:=1;

For j:=1 Step 1 Until M Do Begin
If EVEN Then Else Goto ODD;
   J1:=j;   J2:=j+1;    JJ:=j;
   WALL:=HALF:=j=M;
   Goto L1;
ODD:J1:=j-1;    J2:=j;    JJ:=j-.5;
   HALF:=JJ < 1.;
   WALL:=j=M;
L1: If WALL Then JJ:=M1;
If HALF Then Begin
   If WALL Then Begin
   Cin[j]:=C[J1];
   Tin[j]:=T[J1];
   End Else Begin
   Cin[j]:=C[J2];
   Tin[j]:=T[J2];
End End Else Begin
Cin[j]:=((JJ-.75)*C J1 +(JJ-.25)*C[J2])/(2.*JJ-1.);
Tin[j]:=((JJ-.75)*T J1 +(JJ-.25)*T[J2])/(2.*JJ-1.);
End;
```

```
Stage (Cin[j], Tin[j], Cout[j], Tout[j], Rate[j], K0, flux,
       WALL, HALF, M1, DELTA[i, j]);
End of one row;
Cave:=0;
Tave:=0;
For j:=1 Step 1 Until M Do Begin
Cave:=Cave+Area[ONE, j]*Cout[j];
Tave:=Tave+Area[ONE, j]*Tout[j];
C[j]:=Cout[j];
T[j]:=Tout[j];
End;
PRINT (F12, i, flux, Cave, Tave);
If   SLON(2) Then Begin
PRINT(F21, C[1], ... , C[M]);
PRINT(F22, T[1], ... , T[M]);
End;
If SLON (1) Then PRINT(F23, For j:=1 Step 1 Until M Do DELTA[i,j]);
End of procedure;

Program 206;
Begin
Comment To prepare the 'factor' matrix for program 200;
Real K0;
Integer i,j;
Real Array factor, T, Rate[0:6], TW, flux[0:58], Area[0:1, 1:6],
          DELTA[1:113, 1:5];
```

```
McProcedure Row (205, 1, 13);
Format F1(J2, 6(S2, R5));
For j:=1 Step 1 Until 5 Do Begin
factor[j]:=0;
T[j]:=1.;
End; factor[5]:=1.;
K0:=1.035; If SLON (13) Then K0:=1.;
PUNCH (For j:=1 Step 1 Until 5 Do factor[j]);
PRINT (F1, For j:=1 Step 1 Until 5 Do factor[j]);
For i:=3 Step 1 Until 113 Do Begin
For j:=1 Step 1 Until 5 Do factor[j]:=K0*factor[j];
Row (i, 5, 4.5, factor, T, 1., 0, Area, Rate, 0, DELTA);
If i=3 Then factor[5]:=K0 Else factor[5]:=0;
PUNCH (For j:=1 Step 1 Until 5 Do factor[j]);
PRINT (F1, For j:=1 Step 1 Until 5 Do factor[j]);
End End;
```