

SYSTEM ANALYSIS AND OPTIMIZATION STUDY OF
A MULTISTAGE GAS COMPRESSION SYSTEM

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CHAPTER 1. INTRODUCTION

1. Application of Modern Optimization Theory to Practical Processes

Optimization theory deals with achieving the best--maximum gain or minimum loss--in a rational manner. This holds great interest for the practical professions of engineering. Spectacular advances have been made in optimization theory producing a massive, jargon-filled literature on linear, non-linear and dynamic programming, the maximum principle and many other optimization techniques. In the meantime, electronic computers have been developed with enormous computational speed and large memory capacities. With the extensive developments in these two fields, the time has come when modern optimization theory can be applied to find optimum policies for complicated practical processes.

Movement along this line has already been initiated at the Kansas State University and several papers have already been published (1, 2, 3, 4). The present study has been undertaken to contribute to this move. A multistage gas compression process is a well-known process of great practical importance. In this study, system analysis is applied to multistage gas compression, and the discrete analog of the maximum principle is used to find the optimal policies and numerical computations have been made for CO_2 gas compression under various discharge conditions for illustration.

It is hoped that by showing practical applications of modern optimization theories, the practicing engineers will be induced to apply the modern theories to problems of their interests.

2. Multistage Gas Compression

Gas compression is very common in chemical process industries. High pressures are needed to obtain an improved equilibrium condition for a separation process, to obtain an improved yield in a chemical process, to attain a high reaction rate, to suppress side reactions, and simply to overcome pressure drop due to friction in transmission lines.

For several reasons the ratio of the discharge pressure to the suction pressure for a single-stage compressor is limited (5). One reason is related to the efficiency of operation. Figure 1 illustrates the compression process for adiabatic (1-2) and isothermal (1-3) paths. The work required in the adiabatic compression is represented by area 1-2-8-7 and the work required in the isothermal compression is represented by area 1-3-8-7. Therefore, the isothermal process requires less work than the adiabatic process by an amount equivalent to the area 1-2-3. Actually the compression step is more nearly adiabatic than isothermal, since it is impossible to transfer a large quantity of heat through the cylinder walls in the short time accompanying the stroke of the piston. Nevertheless, the benefits of isothermal operation can be partly achieved by dividing the process into two steps, that is, by limiting the discharge pressure from the first compressor cylinder to P_B , cooling the gas to the original temperature t , in an intercooler (a process occurring at essentially constant pressure, path 4-5), and finally completing the compression to P_C in a second cylinder. In this two-stage system a reduction of work equal to the area 2-4-5-6 is accomplished. A further decrease in the work requirement would be obtained by increasing the number of stages to three or

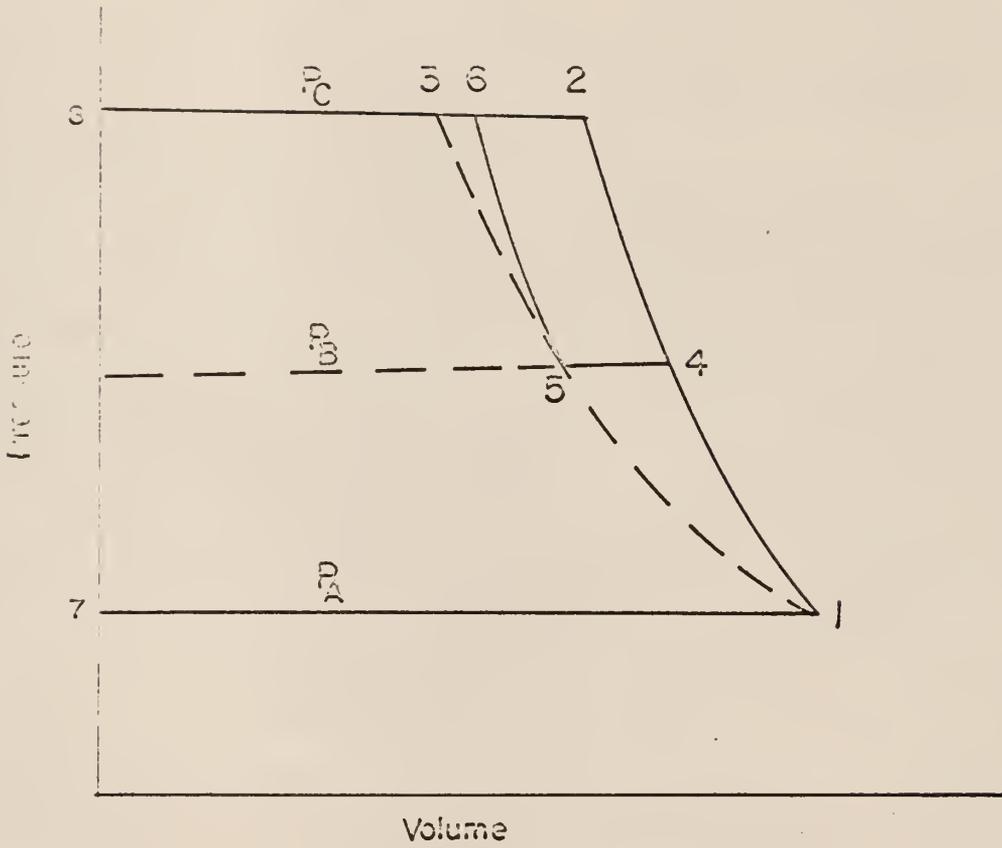


Fig. 1. Comparison of single and two-stage compression operation.

more. However, the maximum reduction in work is limited to the area 1-2-3; hence a point is soon reached at which the decrease in power costs is balanced by the increased first cost of the equipment. The number of stages employed in practice depends primarily upon the overall pressure differential and the capacity. In large machines the pressure ratio per stage is seldom more than 5 or 6 and may be less. In small compressors, where power costs are of less importance, this ratio may be considerably higher.

Very high-pressure machines operating with discharge pressures of the order of 10,000 psia are usually built with five or more stages. As the pressure is increased, the specific volume of the gas decreases and consequently the cylinder size necessary for a given capacity decreases. This is another important reason why high compression ratios are not justified with single-stage machines; large cylinders would be required to handle the low-pressure intake gas, and the entire cylinder would have to be of expensive construction to withstand the high-pressure existing at the end of the stroke.

The efficiencies of reciprocating compressors generally are between 70 and 90 per cent. This means that the actual work required is 11 to 43 per cent greater than computed on the basis of reversible adiabatic operation.

3. The Conventional Methods Used in Optimizing A Multistage Gas Compression System

The conventional methods used in finding the optimal policy of a multistage gas compression system are based on the following assumptions:

- (1) Gas compression in each stage is reversible and adiabatic.

- (2) Gas is cooled to the original temperature after each compression.
- (3) The objective function to be minimized is the total energy used in the gas compression. The first costs of compressors, heat exchangers, and pumps and the operational costs such as cooling water cost are not included in the objective function.

The work required in the multistage gas compression is mostly calculated on the assumption that the gas behaves ideally. Several approaches have been proposed to calculate the compression work requirement for a non-ideal gas.

However, the author is not aware of any publication in which non-ideal gas behavior is taken into account in the optimization study.

The prior work directed to this problem is briefly reviewed as follows:

- a) For ideal gases.

The optimal policy arrived at is to allocate the interstage pressures in such a way as to have an equal horsepower requirement per stage. This criterion gives rise to the optimal policy of allocating the interstage pressures as the geometric means between the suction and discharge pressures.

Derivations leading to the above conclusion are presented in most thermodynamic books. They are mostly based on differentiating the equation of the total energy requirement for the N-stage compression. As an example, the formulation given by Happel (6) is outlined as follows. Under the assumptions described earlier in this section, the

total energy used per mole in the N-stages gas compression is given by

$$E_N = RT \frac{\gamma}{\gamma-1} \left[\left(\frac{P_1}{P_2} \right)^{\frac{\gamma-1}{\gamma}} + \left(\frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}} + \dots + \left(\frac{P_N}{P_{N-1}} \right)^{\frac{\gamma-1}{\gamma}} - N \right] \quad (1)$$

By defining the compression ratios

$$r_{i+1} = \frac{P_{i+1}}{P_i} \quad i = 0, 1, 2, \dots, N-1, \quad (2)$$

and the constants

$$nRT \frac{\gamma}{\gamma-1} = K \quad (3)$$

$$\frac{\gamma}{\gamma-1} = \alpha^{-1} \quad (4)$$

so that Equation (1) becomes

$$E_N = K \left\{ \sum_{i=1}^N r_i^{\alpha} - N \right\} \quad (5)$$

Happel (6) sought to minimize E_N through appropriate choice of the quantities r_i , $i = 1, 2, \dots, N$, subject to the following constraints:

$$r_1 \geq 1, \quad i = 1, 2, \dots, N \quad (6)$$

$$\prod_{i=1}^N r_i = \Gamma = \frac{P_N}{P_0} \quad (7)$$

and solved this problem for the case $N = 3$, making use of methods of differential calculus.

L. T. Fan and C. S. Wang (7, 7a) have shown that the discrete analog of the maximum principle can be applied to solve this problem. They defined state variables, x_1^n and x_2^n , and a decision variable, θ^n as follows:

x_1^n = pressure of the gas at the end of the n-th stage compression.

x_2^n = work spent in compressing m moles of the gas up to and including the n-th stage compression

$$\theta^n = x_1^n / x_1^{n-1}.$$

They have then shown that the process can be described by the performance equations,

$$x_1^n = x_1^{n-1} \theta^n, \quad x_1^0 = P_0, \quad x_1^N = P_N \quad (8)$$

$$x_2^n = x_2^{n-1} + mRT \frac{\gamma}{\gamma - 1} [(\theta^n)^{(\gamma-1)/\gamma} - 1], \quad x_2^0 = 0 \quad (9)$$

They have recognized that the process as represented by equations (8) and (9) belongs to the one dimensional linear process and then concluded that the optimum condition is represented by

$$\theta^1 = \theta^2 = \theta^3 \quad .$$

This means the optimal increment of pressures at each stage corresponds to the geometric means between the suction and discharge pressures. Fan and Wang (25) have initiated the work on the optimal compression of non-ideal gases.

R. Aris, R. Bellman and R. Kalaba (8) have solved this problem by using the functional-equation technique of dynamic programming, which reduces the N-dimensional optimization to a sequence of N one-dimensional

optimizations. Then they have pointed out the relationship to the well-known arithmetic-geometric mean inequality, and finally they have discussed some generalizations.

b) For non-ideal gases.

R. Aris, et al. (8) have described how a more realistic model can be set up, but have not actually formulated the problem. They suggested that the cost of compression in each stage, denoted as $f(T,P)$, be determined empirically and the optimum condition be found by a search technique utilizing the condition of optimality.

R. York (9) has described ways of computing the work requirement for compressing a non-ideal gas. To allow for gas law deviations, the designer of gas compressors has a choice of two alternatives. The first is to retain the expression obtained for an ideal gas and to add suitable correction factors. The second alternative is to discard the expression for ideal gases and to determine the enthalpy change at constant entropy between the states existing within the compressor cylinder. These two fundamental properties of enthalpy and entropy are presented in tables of thermodynamic properties or graphed as a Mollier diagram. York has adopted the first approach and proceeded to show that in order to allow for deviations from the perfect gas law, two correction factors are needed. The first is a correction for volume, which can be expressed in terms of the compressibility factor. The second is a correction for the enthalpy change $(\Delta H)_s$ along an isentropic path of compression and is termed the "isentropic work factor". He has then shown a figure for the isentropic work factor for propane, but has not generalized it.

Other methods purporting to allow for gas law deviations have been proposed. The first of these is by Lavery (10). He has pointed out that gas law deviations affect only the quantity of gas aspirated per stroke with a given cylinder. Furthermore, he has stated: "It (the compressor) has no way of correcting for the deviations of the gas laws, and if the gas is more dense, it is compressed with no increase in horsepower." Both these statements are based upon the fact, as is the practice, that gas quantities are reported as volumes at measuring pressure P_0 (usually 14.7 psia) and at suction temperature. The statement regarding the gas aspirated is without doubt true. The quoted statement regarding the power requirement is only partly true--it does not tell the whole truth! Actually the power requirement is decreased. In an example to illustrate the correction for gas law deviations, Lavery shows that, for a given volume of gas at P , the brake horsepower for an imperfect gas is decreased by the compressibility factor μ . Since μ is a volume correction only, it cannot directly affect the horsepower. The power correction should be made along an isentropic path of compression and not at one point for the volume.

The second method to allow for gas law deviations was proposed by Edmister (11). By his method the ratio c_p/c_v , here denoted by k , is corrected for gas law deviations. This corrected ratio was presented graphically as a generalized correlation in terms of reduced pressure and reduced temperature. A study of his plot shows that k at any pressure and temperature is always greater than k at zero pressure, the state of a perfect gas. Such values of k necessarily give greater power requirements than for a perfect gas. Unfortunately the reverse is true--the power requirement decreases! His correlation is satisfactory

for presenting values of k but unsatisfactory in the applications mentioned. It must be remembered that, if a gas deviates from a perfect gas in its P-V-T relations, it will deviate in all its thermodynamic properties, including enthalpy and entropy.

4. The Special Features of the Present Study

The primary objective of this study is to improve the system analysis and optimization study of a multistage gas compression system. In this study most of the inadequacies of the conventional methods have been removed. The special accomplishments in this study are summarized as follows:

- (a) An improved system analysis is made and an objective function more realistic than the one used in the conventional approach is obtained. The unrealistic assumptions made in the conventional methods have been removed. In this study, we take into consideration the non-ideal behavior of a gas and irreversibilities of the compressors. The first costs of the compressors, inter-stage coolers and pumps, the cooling water cost, and energy cost are included in the objective function.
- (b) A generalized treatment is made so that the relations obtained and even the computer program established can be readily applied to any gas under any operating conditions by simply replacing input data sheets. A generalized equation of state and the generalized thermodynamic excess functions developed by Hirshfelder et al. (12, 13) have been used in the system analysis. Therefore, the equations obtained are applicable to practically all gases.

- (c) An efficient computational scheme is established and a step-by-step description of the iterative numerical computation is given. This is done in such a way that average engineers can easily follow the procedure to apply the method to the problems of their interest.
- (d) It is demonstrated that the discrete analogue of the maximum principle is very powerful in handling a multistage optimization problem of high dimensionality, even though it does not always give rise to an absolute optimum. The optimization problem formulated in this study has six decision variables, seven state variables in each stage together with four equality constraints.
- (e) Numerical computations have been actually carried out for three stage CO₂ gas compression under various discharge conditions. The results obtained demonstrate the practical importance of this study by showing the cost reduction realizable by this method as compared with the conventional methods.

CHAPTER 2. PROCESS ANALYSIS OF A MULTISTAGE GAS COMPRESSION SYSTEM

1. Introduction

In this chapter, a system analysis is made for a multistage irreversible compression of a non-ideal gas with arbitrary interstage cooling. The gas is not necessarily cooled to the original temperature after each compression as is usually assumed. A realistic objective function which conforms to the industrial practice is formulated.

In the analysis, several thermodynamic functions at each stage have been introduced. These are the entropies of the gas after a hypothetical reversible compression and after the interstage cooling, enthalpies of the gas after a hypothetical reversible compression, after an actual compression and after interstage cooling and the cumulative cost of the gas compression up to the stage. The work required in the compression and the heat load for the intercoolers are found.

In order to establish performance equations in the form convenient for the application of the discrete analog of the maximum principle, the enthalpy, entropy, cumulative cost, and pressure have to be related to the respective temperature and density. The generalized equation of state and generalized thermodynamic excess functions will be obtained, and the optimization problem will be set up in the final form in Chapter 4.

2. Process Description

Figure 2 illustrates a general multistage (N-stage) gas compression system with interstage cooling. Each stage (say the n-th stage) consists

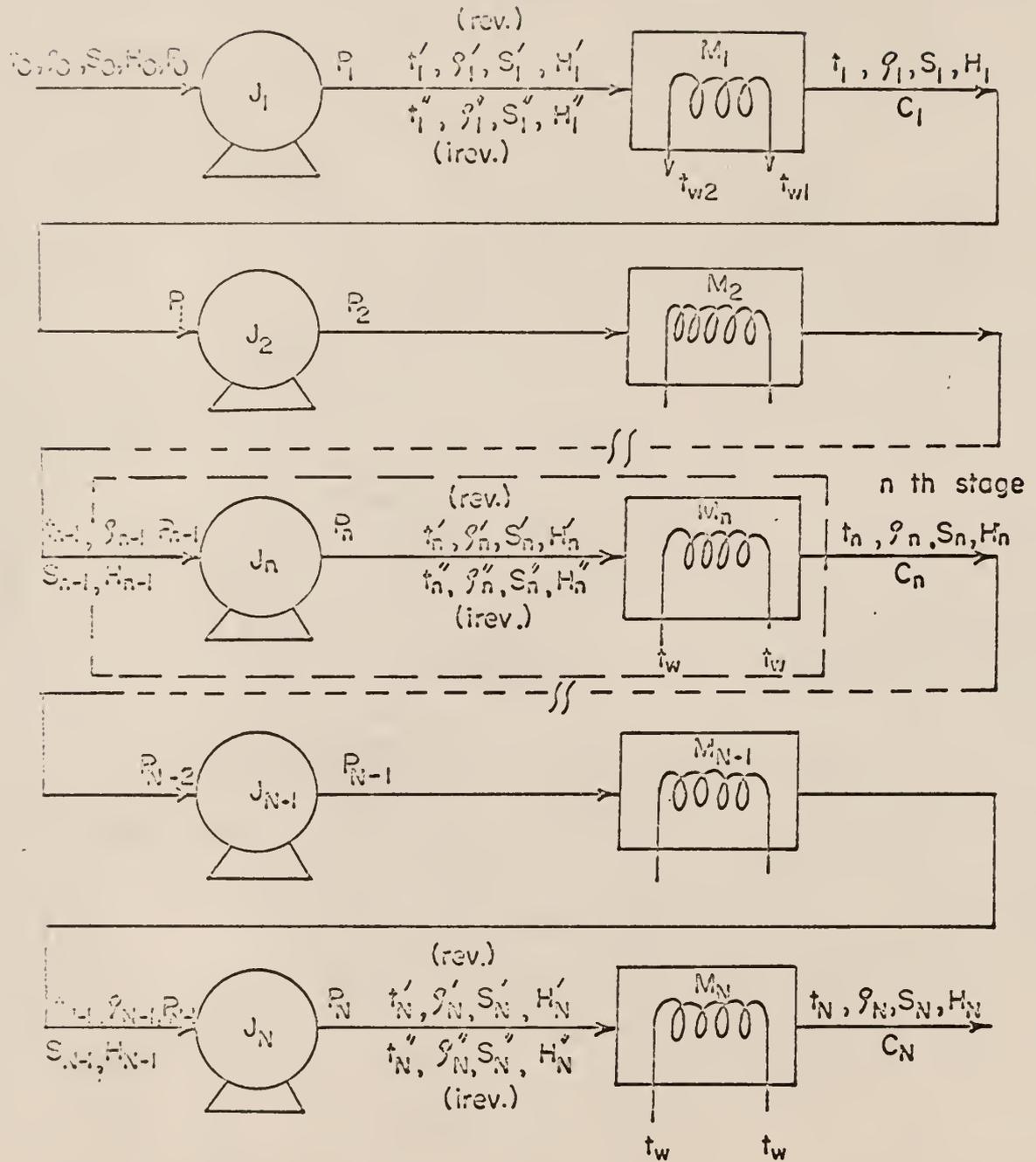


Fig. 2. Multistage compression with interstage cooling.

of a gas compressor J_n and an intercooler M_n . In a multistage gas compression system, the feed gas flows through the successive stages and is compressed and cooled alternatively. The usual assumption of cooling to the original temperature is removed in this analysis and the temperature to which the gas is cooled in each stage is considered as a control variable.

The following notations are used in subsequent discussions:

P_0, P_n, P_N = respectively, pressure of the feed gas, pressure of the gas in the n-th stage and the pressure at the last stage, or equivalently, the discharge pressure, in psia.,

T_0, T_n, T_N = respectively, temperature of the feed gas, temperature of the gas leaving the n-th stage and the temperature of the gas discharged from the system in °F.,

t_0, ρ_0, S_0, H_0 = respectively the reduced temperature, the reduced density, the entropy per lb-mole, the enthalpy per lb-mole of the feed gas.

$t'_n, \rho'_n, S'_n, H'_n$ = respectively, the reduced temperature, the reduced density, the entropy per lb-mole, the enthalpy per lb-mole of the gas after a hypothetical (reversible) compression in the n-th stage

$t''_n, \rho''_n, S''_n, H''_n$ = respectively, the reduced temperature, the reduced density, the entropy per lb-mole, the enthalpy per lb-mole of the gas after an actual (irreversible) compression in the n-th stage,

t_n, ρ_n, S_n, H_n = respectively, the reduced temperature, the reduced density, the entropy per lb-mole, the enthalpy per lb-mole of the gas after the n-th stage cooler M_n

C_n = cumulative gas compression cost up to and including the n-th stage,

C_N = cumulative gas compression cost up to and including the last stage.

Referring to the n-th stage of the system, a gas stream (characterized by $t_{n-1}, \rho_{n-1}, S_{n-1}, H_{n-1}$) is pressurized by an actual compressor J_n from a pressure P_{n-1} to a pressure P_n and the gas leaving the compressor is characterized by t_n'', ρ_n'', S_n'' and H_n'' . After being cooled by a cooler M_n , the gas properties become t_n, ρ_n, S_n and H_n . Assuming a hypothetical reversible compression in J_n , the gas leaving the compressor would have been characterized by t_n', ρ_n', S_n' and H_n' . The properties of this hypothetical gas stream are needed as linking properties which are useful in evaluating actual compression.

It is assumed in this study that the cooling water enters each cooler at the same temperature $(t_w)_i$ and leaves at the same temperature $(t_w)_o$. $(t_w)_i$ is fixed in a chemical plant as the water temperature from a cooling tower or a cooling pond. In a chemical plant, cooling water is generally regenerated and recycled within the plant and has a rather high dissolved solid content. Therefore, $(t_w)_o$ is limited to about 110° F to prevent scale formation. In a future study $(t_w)_o$ may be considered as a control variable which may be different in each stage.

3. Process Analysis - Relations Among the Operating Variables

Referring to the n-th stage of Figure 2, the following relations can be established.

- (a) Entropy is unaltered during a reversible adiabatic compression. Therefore, we have

$$S_{n-1} = S'_n \quad (1)$$

- (b) The work of compression in a hypothetical reversible compression is given by

$$W_{\text{rev}} = (\Delta H_n)_s = H'_n - H_{n-1} \quad (2)$$

- (c) The work of compression in an actual compression is given by

$$W_{\text{irr}} = (\Delta H_n)_a = H''_n - H_{n-1} \quad (3)$$

- (d) The efficiency of the compression, η , is defined as

$$\eta = \frac{W_r}{W_{\text{irr}}} = \frac{H'_n - H_{n-1}}{H''_n - H_{n-1}} \quad (4)$$

This gives rise to

$$(H''_n - H_{n-1}) = \frac{1}{\eta} (H'_n - H_{n-1}) \quad (5)$$

The η value ranges from 70% to 90%. In the latter calculation η will be taken as $\frac{1}{1.2}$.

- (e) The heat to be removed in the cooler M_n is given as

$$q = -\Delta H = H''_n - H_n \quad (6)$$

(f) The heat transfer area, Λ_n , required is given by

$$\Lambda_n = \frac{q}{U \Delta T} = \frac{H_n'' - H_n''}{U T_c \left[(t_1 - t_1) - (t_1' - t_2') \right]} \ln \frac{t_1 - t_2}{t_1' - t_2'} \quad (7)$$

where t_1 , t_2 are respectively temperatures in reduced unit of the gas and the cooling water at one end of the heat exchanger and t_1' and t_2' are respectively temperatures in reduced unit of the gas and the cooling water at the other end of the heat exchanger.

4. A Mathematical Model for a Multistage Gas Compression System

In optimizing any system, the operating variables may be classified into decision variables and state variables. Denoting a state variable associated with the n-th stage as X_i^n and denoting a decision variable associated with the n-th stage as θ_i^n , for a system represented by a set of finite difference equation, X_i^n can be expressed as

$$X_i^n = F_i^n(X_1^{n-1}, X_2^{n-1}, \dots, X_5^{n-1}, \theta_1^n, \theta_2^n, \dots, \theta_t^n) \quad (8)$$

That is, X_i^n is a function of state variables associated with the (n-1)-th stage and the decision variables of the n-th stage. The above equation is called the performance or transition equation for X_i^n ,

The operating variables shown in Figure 2 are classified into decision and state variables as follows:

(a) decision variables:

$$\begin{aligned} \theta_1^n &= t_n', & \theta_2^n &= t_n'', & \theta_3^n &= t_n \\ \theta_4^n &= p_n', & \theta_5^n &= p_n'', & \theta_6^n &= p_n \end{aligned} \quad (9)$$

(b) state variables:

$$\begin{aligned}
 x_1^n &= p_n, & x_2^n &= H_n', & x_3^n &= H_n'', & x_4^n &= H_n \\
 x_5^n &= S_n', & x_6^n &= S_n, & x_7^n &= C_n,
 \end{aligned}
 \tag{10}$$

Figure 3 shows the structure of the finite difference or discrete model. Decision variables are shown in association with vertical arrows, and state variables are shown in association with horizontal arrows. The constraint functions ϕ_i^n shown in the figure will be explained shortly.

5. The Performance Equations and the Degree of Freedom

With the above classification, it will be shown that all the state variables can be expressed as follows:

State - space notation	conventional notations
$x_1^n = T_1^n(\theta_1^n, \theta_4^n)$	$p_n = f_1(t_n', \rho_n')$
$x_2^n = T_2^n(\theta_1^n, \theta_4^n)$	$H_n' = f_2(t_n', \rho_n')$
$x_3^n = T_3^n(\theta_2^n, \theta_5^n)$	$H_n'' = f_3(t_n'', \rho_n'')$
$x_4^n = T_3^n(\theta_3^n, \theta_6^n)$	$H_n = f_4(t_n, \rho_n)$
$x_5^n = T_5^n(\theta_1^n, \theta_4^n)$	$S_n' = f_5(t_n', \rho_n')$
$x_6^n = T_6^n(\theta_3^n, \theta_6^n)$	$S_n = f_6(t_n'', \rho_n'')$
$x_7^n = T_7^n(\theta_2^n, \theta_3^n, \theta_5^n, \theta_6^n;$ $x_4^{n-1}, x_7^{n-1})$	$C_n = f_7(t_n'', t_n, \rho_n'', \rho_n;$ $H_{n-1}, C_{n-1})$

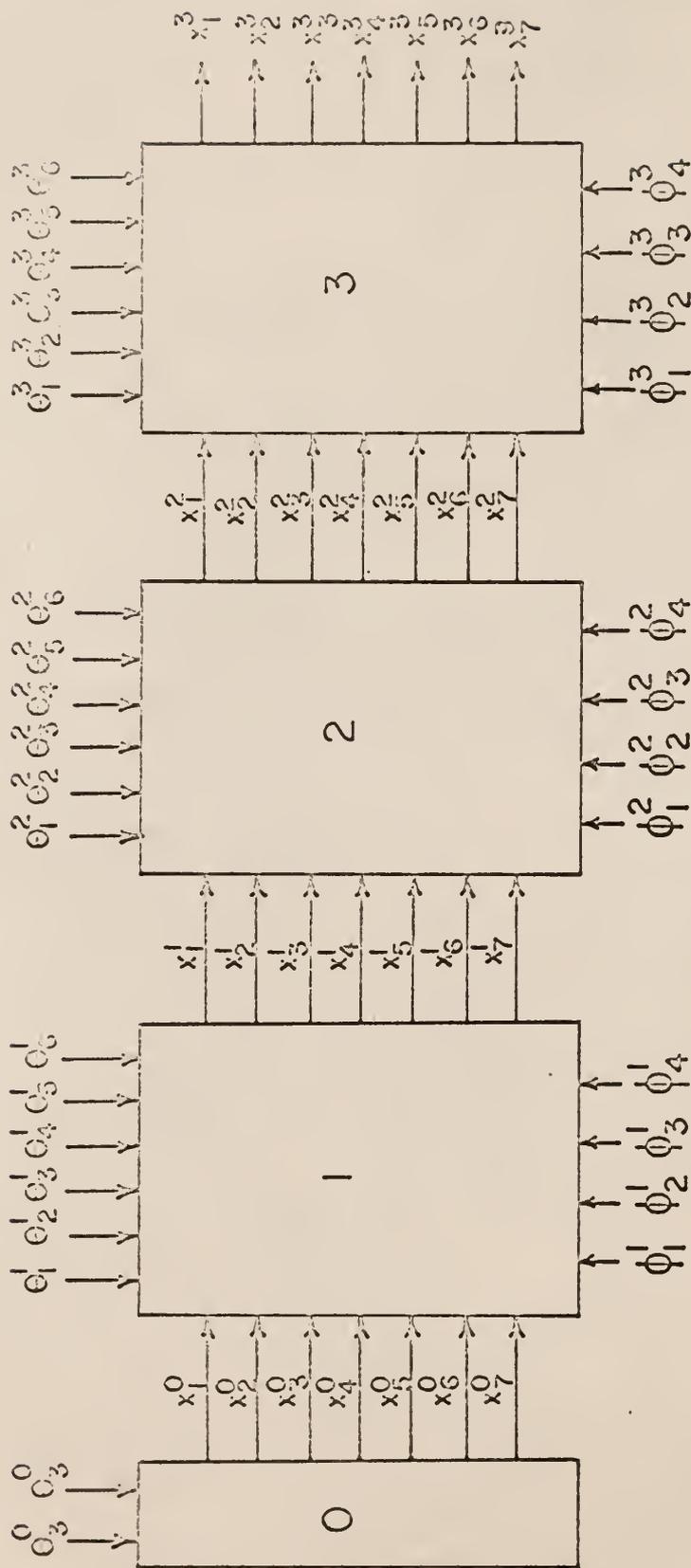


Fig 3. The stagewise model of a multistage gas compression system .

It is seen that the above performance equations do conform to the form of equation (8). Explicit expressions for these equations will be derived at the end of the next chapter.

In addition to the above performance equations, the following relations which become equality constraints in the n-th stage must be considered.

1. Pressure at the n-th stage is considered to be constant. That is, pressure of the gas after the hypothetical (isentropic) compression, pressure of the gas after the actual compression, and the pressure after the cooler are the same. Therefore, one has

$$P_n = f_1(t_n', \rho_n') = f_1(t_n'', \rho_n'') = f_1(t_n, \rho_n) \quad (12)$$

The equality constraint functions, ϕ_1^n and ϕ_2^n are defined as

$$\phi_1^n = f_1(t_n', \rho_n') - f_1(t_n'', \rho_n'') = 0 \quad (13)$$

$$\phi_2^n = f_1(t_n', \rho_n') - f_1(t_n, \rho_n) = 0 \quad (14)$$

These equations can be written in maximum principle notations as

$$\phi_1^n = T_1^n(\theta_1^n, \theta_4^n) - T_1^n(\theta_2^n, \theta_5^n) = 0 \quad (15)$$

$$\phi_2^n = T_1^n(\theta_1^n, \theta_4^n) - T_1^n(\theta_3^n, \theta_6^n) = 0 \quad (16)$$

2. During an reversible compression, the entropy value is unchanged.

Therefore, one has

$$S_n' = S_{n-1} \quad (17)$$

The equality constraint function ϕ_3^n is defined as

$$\phi_3^n = S_n' - S_{n-1} = 0 \quad (18)$$

This equation can be written in state-space notation as

$$\begin{aligned} \phi_3^n &= x_5^n - x_6^{n-1} \\ &= T_5^n(\theta_1^n, \theta_4^n) - x_6^{n-1} \\ &= 0 \end{aligned} \quad (19)$$

3. The compressor efficiency equation is given as

$$(H_n'' - H_{n-1}') = \frac{1}{\eta}(H_n' - H_{n-1}) \quad (20)$$

The equality constraint function ϕ_4^n is defined as

$$\phi_4^n = (H_n'' - H_{n-1}') - \frac{1}{\eta}(H_n' - H_{n-1}) = 0 \quad (21)$$

This equation can be written in state-space notation as

$$\phi_4^n = (x_3^n - x_4^{n-1}) - \frac{1}{\eta}(x_2^n - x_4^{n-1}) = 0 \quad (22)$$

State variables are dependent variables as expressed by equation (11). Out of the six decision variables in each stage only two are truly independent due to the four equality constraints shown above.

In a multistage gas compression problem, the temperature and pressure of the gas discharged from the last stage are usually pre-assigned values. Due to these two additional constraints, the degree of freedom of a multistage (N stages) gas compression system becomes $2(N-1)$.

6. Mapping of a Multistage Gas Compression Operation on a H-S Diagram

The operation of a multistage gas compression operation can best be illustrated on either the T-S or the H-S diagram for the gas. The operation of a three-stage compression of CO₂ gas from pressure P₀ (= 14.7 psia) and temperature T₀ (= 545° R) to the final condition of pressure P₃ (= 1700 psia) and temperature T₃ (= 600° R) by realistic compressors J₁, J₂ and J₃ and coolers M₁, M₂ and M₃ is illustrated by the path (1)-(3)-(4)-(6)-(7)-(9)-(10) in the Figure 4, which is the T-S diagram for CO₂(14).

The steps (1)-(3), (4)-(6) and (7)-(9) correspond to gas compressions by J₁, J₂ and J₃ respectively and the steps (3)-(4), (6)-(7) (9)-(10) correspond to gas coolings by M₁, M₂, and M₃ respectively. The construction of these steps is explained as follows:

a) Realistic gas compression step.

Take step (1)-(3) for example. The feed gas is compressed from P₀ to P₁ and point (2) can be located as follows:

- 1) Locate point (1) corresponding to the feed gas condition P₀, T₀,
- 2) Locate point (2) by following a constant entropy line from point (1) until it hits the constant pressure line with pressure P₁. This point corresponds to the condition of the gas after a hypothetical reversible compression to pressure P₁.

3) Locate point (3) by the following two conditions

- i. point (3) lies on the constant pressure line at P₁

- ii.
$$\frac{H(\text{at point (3)}) - H(\text{at point (1)})}{H(\text{at point (2)}) - H(\text{at point (1)})} = \frac{1}{\eta}$$

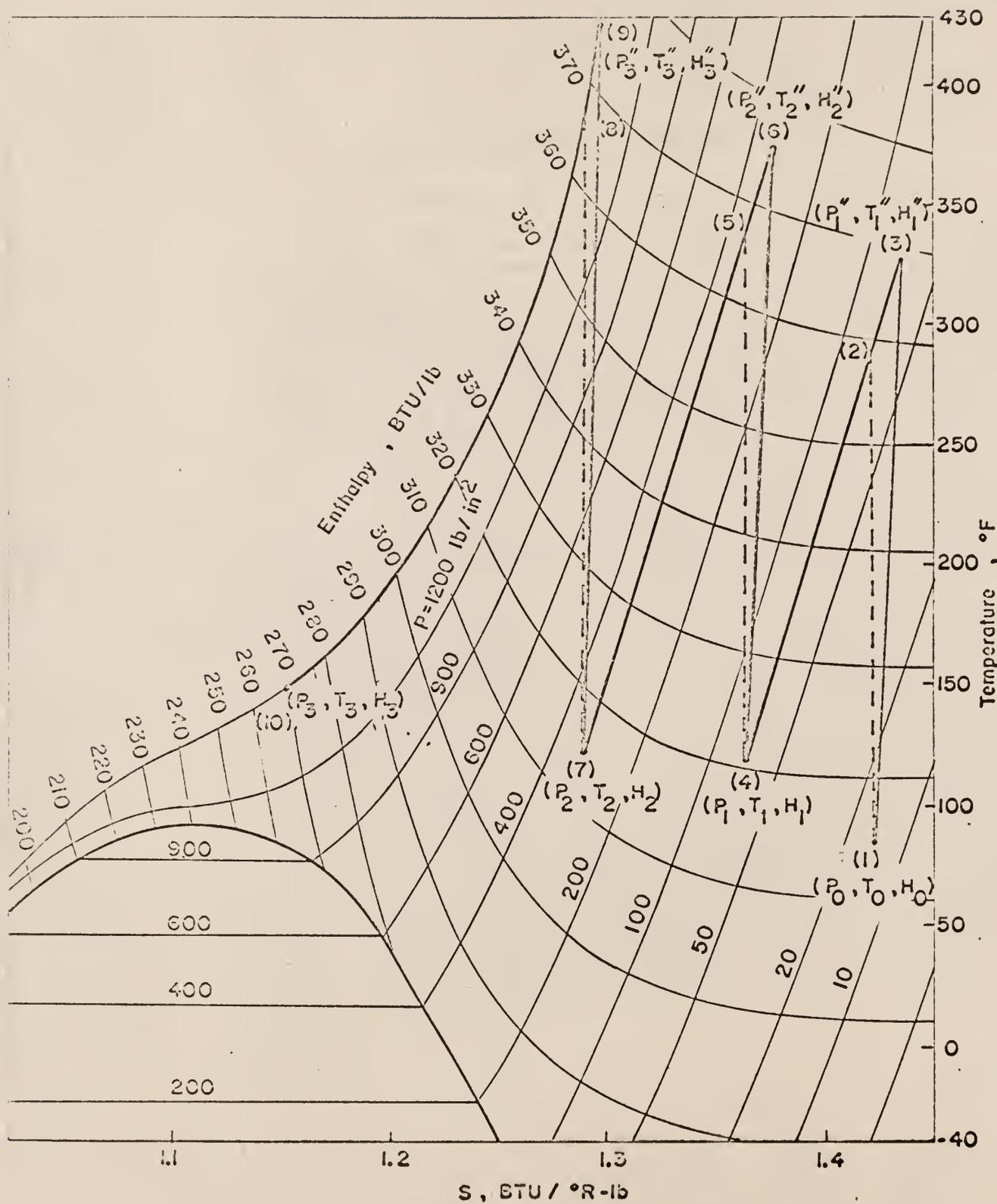


Fig. 4. Liquid-vapor-temperature-entropy diagram for carbon dioxide.
(14)

Other compression steps (4)-(6) and (7)-(9) can be similarly constructed.

b) Gas cooling steps.

Temperatures of the gas leaving the coolers M_1 and M_2 are independent variables. In the optimization study, these two temperatures will be controlled together with other control variables to arrive at the optimum policy.

Once T_1 and T_2 are given point (4) and (7) can be located as corresponding to the conditions (P_1, T_1) and (P_2, T_2) respectively. Point (10) corresponds to the final condition of the gas. The cooling steps (3)-(4), (6)-(7), and (9)-(10) are on constant pressure lines.

7. Gas Compression Cost

The gas compression cost may be considered to be consisting of the cost of the work of compression at each stage, E_1^n 's; costs allocated to the gas due to the initial costs of the compressors, E_2^n 's; costs allocated to the gas due to the intercoolers at each stage, E_3^n 's; and the costs of cooling water used in individual stages, E_4^n 's.

Referring to Figure 4, the work of compression and the enthalpy change in the intercooler at the n-th stage are $(H_n'' - H_{n-1})$ and $(H_n'' - H_n)$ respectively. Assuming that the compressor cost and intercooler cost are proportional to the power and the heat transfer area respectively, the cost spent for compressing 1 lb-mole of the gas at the n-th stage is given by

$$\sum_{i=1}^4 E_i^n = E_1^n + E_2^n + E_3^n + E_4^n$$

$$\begin{aligned}
&= C_e (H_n'' - H_{n-1}) + \psi_1 C_{HP} (H_n'' - H_n) \\
&+ \frac{\psi_2 C_H}{U \cdot T_c} \cdot \frac{(H_n'' - H_n)}{[t_n'' - (t_w)_o] - [t_n - (t_w)_i]} \ln \frac{t_n'' - (t_w)_o}{t_n - (t_w)_i} \\
&+ \frac{C_w}{(C_p)_w T_c} \frac{H_n'' - H_n}{(t_w)_o - (t_w)_i} \quad (23)
\end{aligned}$$

where C_e and C_w are respectively unit power cost and unit cooling water cost, C_{HP} and C_H are respectively unit compressor cost and unit heat transfer area cost and ψ_1 and ψ_2 are the fraction of initial costs of the compressor and the intercooler respectively allocated and chargeable to one operation hour and U is the overall coefficient of heat transfer.

CHAPTER 3. GENERALIZED EQUATION OF STATE AND GENERALIZED THERMODYNAMIC EXCESS FUNCTION OF GASES

1. Introduction

As has been described, the primary purpose of the present study is to develop a system analysis and an optimization study for a multi-stage gas compression system which are so general as to be applicable to all gases under ideal as well as highly non-ideal states. Therefore, a generalized equation of state which has a wide application range has to be found. From such a generalized equation of state, generalized thermodynamic excess functions can be derived. It is fortunate that such a generalized equation of state is available.

The generalized equation of state adopted in the present study has been taken from the works of J. O. Hirshfelder, R. J. Buehler, H. A. McGee, Jr., and J. R. Sutton (12). Although countless equations (15, 16, 17) and tables (18) are available for predicting the volumetric and thermodynamic properties of gases, the equations developed by Hirshfelder et al. best suit in the present study.

Hirshfelder et al. (13) have also derived generalized thermodynamic excess functions for gases and liquids by starting from their generalized equation of state. These equations are also utilized in formulating performance equations for this study.

In their formulation of the equation of state, they divide the field into three regions. System analysis and optimization made in this study is limited to region I. But the procedure developed can be applied to cover the whole field.

PART A. EQUATION OF STATE

2. The Special Features of the Generalized Equations of State Developed by Hirshfelder et al.

The equations developed by J. O. Hirshfelder et al. (12) are particularly suitable for the present study for the following reasons:

(1) The framework is believed adequate for practically all pure substances. The equations are based on a modified principle of corresponding states, and are applicable to noble gases, hydrocarbons, and the highly polar substances, water and ammonia.

(2) The application range is wide. The full range of gases and liquids is covered where experimental data exist: temperatures as low as half and as high as three times the critical, densities up to four times the critical; and pressures up to 190 times the critical.

(3) Standard input data required are available for most gases. Standard input data required are: the three critical constants, the normal boiling point, and (for the liquid region only) the density of the saturated liquid at two temperatures. When experimental data are not available, known procedures can be used to estimate them. When extensive data are available, they may be used to modify the equations.

(4) The equations are differentiable and thermodynamic excess functions can be readily derived from them.

(5) The equations of state and all the derived equations can be conveniently computed by a modern high-speed computer.

(6) There are no non-physical discontinuities in the equation of state and in the derived properties. In their work, the P-V-T values have been arbitrarily divided into three regions, but the boundary

conditions are so established that there are no non-physical discontinuities in these equations.

3. The Generalized Equation of State by Hirshfelder et al.

(a) Division of the field into three regions.

In their approach the P-V-T values have been arbitrarily divided into three regions, with different equations applying in each region. Taken together these expressions define a single consistent equation of state for all values of P, V, and T. The arbitrary division is a compromise which makes possible the use of a relatively simple equation at low densities; it is perhaps an esthetic defect, but it is nevertheless a practical way of meeting conflicting requirements. The regions of definition are shown in Figures 5-a and 5-b and are defined by:

- | | |
|------------------------------|---|
| Region I. Gas. | All temperatures; density less than the critical, $\rho \leq 1$. |
| Region II. High Density Gas. | Temperature above the critical, $t \geq 1$; density greater than the critical, $\rho \geq 1$. |
| Region III. Liquid. | Temperature below the critical, $t \leq 1$; density greater than the critical, $\rho \geq 1$. |

It should be noted that t and ρ are reduced temperature and reduced density respectively. At the junction ($\rho = 1$) between Regions I and II, the pressure, its first and second derivatives with respect to density, and all its derivatives with respect to temperature, are continuous. At the junction ($t = 1$) between Regions II and III, the

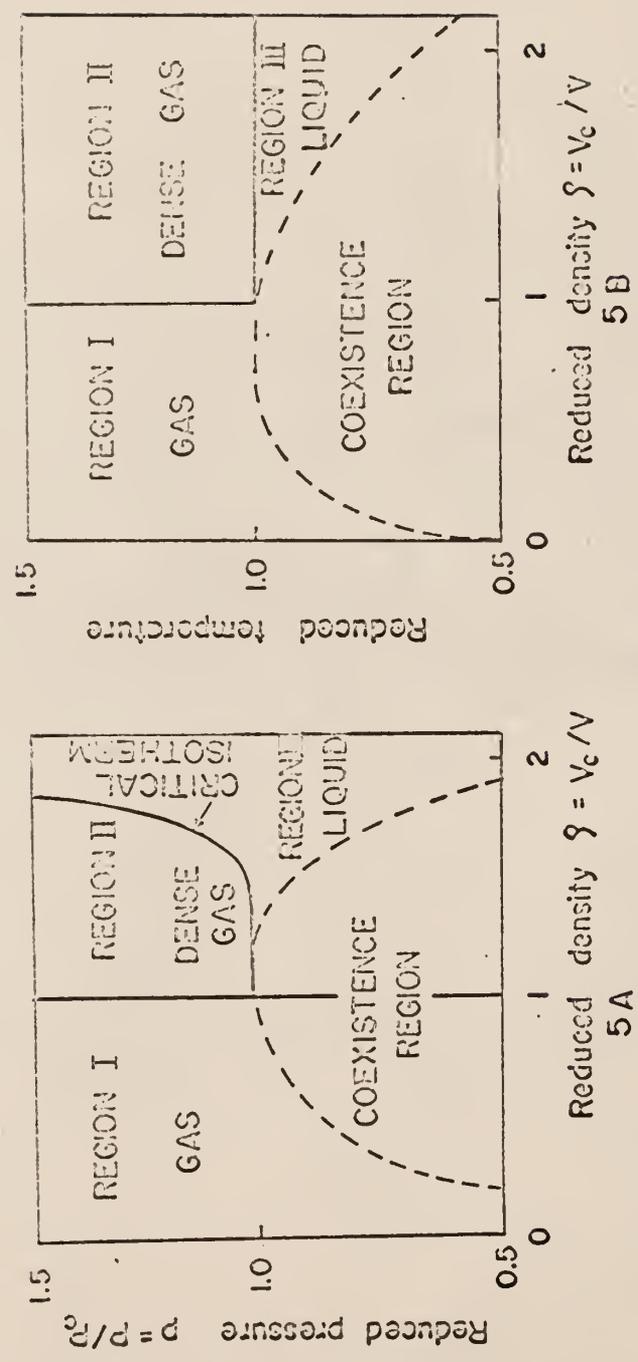


Fig. 5. Regions of definition of equation of state .

pressure, its first derivative with respect to temperature, and all its derivatives with respect to density, are continuous. As might be expected, these continuity requirements lead to some complications; in Region III, for example, the equation is somewhat more complicated than one would like for a normal liquid because of the required continuity along the critical isotherm.

Figures 5-a and 5-b show that at temperatures lower than the critical there is a coexistence region between the liquid region II and gas region I. On the liquid side this region is bounded by values of p and ρ given parametrically by $p_v(t)$ and $\rho_l(t)$, where $p_v(t)$ is the vapor pressure and $\rho_l(t)$ is the density of the saturated liquid. On the vapor side the boundary is given by $p_v(t)$ and $\rho_v(t)$, where $\rho_v(t)$ is the density of the saturated vapor. The coexistence region can be found by knowing the vapor pressure of the substance, which can be computed by such an equation as derived by Riedel (19). This coexistence region is irrelevant to this study because gas compression in which condensation is to be avoided, is considered.

Compression may be made within a single region, region I, II and III. It may span two regions such as I and II, or II and III. For a very high-pressure compression, it may even span the three regions I, II and III. In the present study, gas compression is limited to region I. However, the procedure developed is general, so that compressions spanning several regions may also be handled.

In the following sections, equations of state will be given for the three regions but the generalized excess thermodynamic functions will be given only for region I. Equations for regions II and III are available in the original reference (13).

(b) Explicit relations for equations of state

The equations of state for the regions I, II, and III are given as follows:

i. Region I. Gas

$$p = - (k_0 + k_1 t^{-1}) \rho^2 + k_2 (-t + t^{-1}) \rho^3 + \frac{(\rho t / z_c)}{(1 - b\rho + b'\rho^2)} \quad (1)$$

ii. Region II. Dense Gas

$$p = p_{II} = p(\rho, t) =$$

$$\sum_{j=0}^3 t^{j-1} [k_{0j} + k_{1j}\rho + k_{2j}\rho^2 + k_{3j}\rho^3 + k_{4j}\rho^4 + k_{5j}\rho^5] / \rho \quad (2)$$

iii. Region III. Liquid

$$p = p_{III} = p(\rho, t) = p_{II}(\rho, t) - p_{II}[\rho_L(t), t] + p_v(t) \quad (3)$$

where

p, ρ, t = respectively reduced pressure, reduced density
and the reduced temperature,

$p_{II}(\rho, t)$ = vapor pressure evaluated by equation (2)
at ρ and t ,

$p_{II}[\rho_L(t), t]$ = vapor pressure evaluated by equation (2)
at reduced temperature t and reduced
density $\rho_L(t)$, where $\rho_L(t)$ is the density
of the saturated liquid at t

$p_v(t)$ = saturated vapor pressure at reduced temp. t .

The constants used in the above equations are defined as follows:

$$b = (1/\beta)(3\beta^2 - 6\beta - 1)/(3\beta - 1),$$

$$b' = (\beta - 3)/(3\beta - 1),$$

$$k_0 = 5.5,$$

$$k_1 = \beta - k_0,$$

$$k_2 = (1 - k_0 - \alpha + 2\beta)/2,$$

The constants, k_{ij} , used in the equations (2) and (3) are given in Table 1 as functions of α , β , and k_0 .

where α and β are defined later.

The saturated vapor pressure can be evaluated by the Riedel's correlation (23)

$$\ln p_v(t) = \alpha \ln t + 0.0838 (\alpha - 3.75)(36 t^{-1} - 35 - t^6 + 42 \ln t) \quad (4)$$

and the reduced density of saturated liquid can be evaluated by Guggenheim's correlation (22)

$$\rho_l(t) = 1 + 1.75 (1 - t)^{1/3} + 0.75 (1 - t) \quad (5)$$

The α value in the above equations can be found either from Figure 6 or by the following equation

$$z_c^{-1} = 3.72 + 0.26 (\alpha - 7) \quad (6)$$

The β value can be found either in Table 2 or by the following equation

$$z_c = \beta (3\beta - 1)(1 + \beta)^{-3} \quad (7)$$

Table 1. Constants k_{ij} for Dense Gas and Liquid Regions (12)

	$j = 0$	$j = 1$	$j = 2$	$j = 3$
$i = 0$	0	$88.5 - 3.12\beta$	$-124.46 + 3.84\beta + 0.363\beta^2$	$44.4 - 5.22\beta$
$i = 1$	0	$-313.3 + 13.42\beta$	$405.3 - 6.58\beta - 1.814\beta^2$	$-133.2 + 15.66\beta$
$i = 2$	0	$408.9 - 21.54\beta$	$-457.7 - 7.8\beta + 3.63\beta^2$	$133.2 - 15.66\beta$
$i = 3$	$5.5 - \beta$	$-237.4 + 15.3\beta$	$191.9 + 25.48\beta - 3.63\beta^2$	$-44.4 + 5.22\beta$
$i = 4$	$-2.25 - \frac{\beta}{2} + \beta$	$47.8 - 4.06\beta$	$\beta/2 - 3.35 - 19.44\beta + 1.815\beta^2$	0
$i = 5$	0	0	$-8.44 + 4.50\beta - 0.363\beta^2$	0

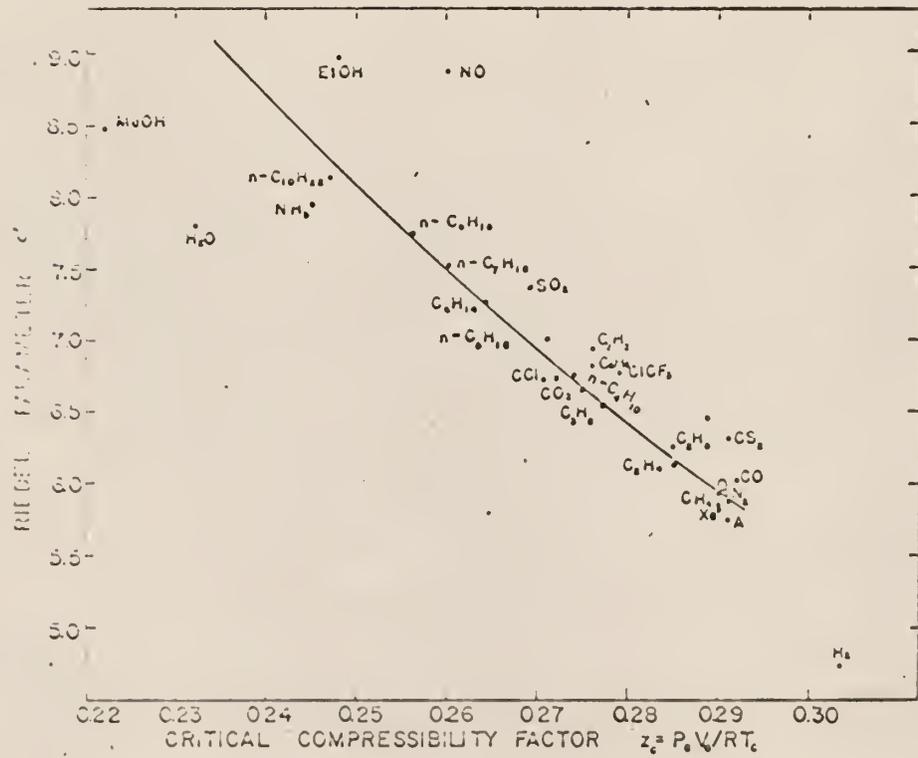


Fig. 6. Comparison of parameters, α and Z_c , for different substances. (12).

Table 2. Parameter β as a Function of z_c (12)

z_c	β	z_c	β
0.230	9.24	0.266	7.34
0.232	9.12	0.263	7.25
0.234	9.00	0.270	7.15
0.236	8.88	0.272	7.06
0.238	8.77	0.274	6.97
0.240	8.65	0.276	6.89
0.242	8.55	0.278	6.80
0.244	8.44	0.280	6.71
0.246	8.33	0.282	6.63
0.248	8.23	0.284	6.54
0.250	8.12	0.286	6.46
0.252	8.02	0.288	6.38
0.254	7.92	0.290	6.30
0.256	7.82	0.292	6.21
0.258	7.72	0.294	6.13
0.260	7.62	0.296	6.05
0.262	7.53	0.298	5.98
0.264	7.43	0.300	5.90

PART B. ENTHALPY AND ENTROPY OF A NON-IDEAL GAS

4. Enthalpy of a Non-Ideal Gas: $H = f_1(\rho, t)$

The thermodynamic excess function for enthalpy utilizing the generalized equation of state developed by Hirshfelder et al. will be derived first and then the enthalpy function will be related to the reduced temperature and the reduced density of the gas.

It is convenient to start from the internal energy function U . It is known that

$$dU = C_v dT + \left[T \left(\frac{\partial P}{\partial T} \right)_v - P \right] dV \quad (8)$$

Under isothermal condition, this leads to

$$dU = \left[T \left(\frac{\partial P}{\partial T} \right)_v - P \right] dV \quad (9)$$

Since

$$p = \frac{P}{P_c}, \quad t = \frac{T}{T_c}, \quad \text{and} \quad \rho = \frac{V_c}{V} \quad (10)$$

One can write

$$P = p P_c, \quad T = t T_c, \quad \text{and} \quad V = \frac{V_c}{\rho} \quad (11)$$

Substituting these relations into equation (9), yields

$$\begin{aligned} dU &= \left[(T_c \cdot t) \frac{P_c}{T_c} \left(\frac{\partial p}{\partial t} \right) - P_c p \right] V_c \frac{(-d\rho)}{\rho^2} \\ &= -P_c V_c \left[t \left(\frac{\partial p}{\partial t} \right) - p \right] \frac{d\rho}{\rho^2} \end{aligned}$$

$$\therefore \frac{U - U_0}{RT} = -\frac{P_c V_c}{R T_c t} \int_0^\rho \left[t \left(\frac{\partial p}{\partial t} \right) - p \right] \frac{d\rho}{\rho^2} \quad (12)$$

where U_0 is the internal energy of the gas at a very low pressure and at the same temperature.

Since t is constant in the integration, and since

$$Z_c = \frac{P_c V_c}{R T_c}$$

equation (12) can be rewritten as

$$\frac{U - U_0}{RT} = Z_c \int \left[\frac{P}{t} - \left(\frac{\partial P}{\partial t} \right) \right] \frac{d\rho}{\rho^2} \quad (13)$$

This equation represents the thermodynamic excess function for the internal energy function.

We can proceed to derive the thermodynamic excess function for enthalpy as follows:

Since

$$H = U + PV,$$

one can write

$$\frac{H - H_0}{RT} = \frac{U - U_0}{RT} + \frac{PV}{RT} - \frac{P_0 V_0}{RT} \quad (14)$$

where H_0 is the enthalpy of the gas at a very low pressure and at the same temperature. Since,

$$Z = \frac{PV}{RT} = \frac{P P_c V_c}{R T_c t \rho} = \frac{P}{\rho \cdot t} \frac{P_c V_c}{R T_c} = Z_c \cdot \frac{P}{\rho t} \quad (15)$$

and

$$\frac{P_0 V_0}{RT} = 1,$$

equation (14) becomes

$$\frac{H - H_0}{RT} = \frac{U - U_0}{RT} + \frac{Z_c p}{\rho t} - 1 \quad (16)$$

By substituting equation (13) into the above equation one obtains

$$\frac{H - H_0}{RT} = Z_c \int_0^{\rho} \left[\left(\frac{\rho}{t} \right) - \left(\frac{\partial p}{\partial t} \right) \right] \frac{d\rho}{\rho^2} + \frac{Z_c p}{\rho t} - 1 \quad (17)$$

This equation represents the thermodynamic excess function for the enthalpy function. H can be related to ρ and t by integrating the above equation.

For a non-idea gas in region I, one can substitute equation (1) into the above equation and obtain

$$\begin{aligned} \frac{H - H_0}{RT} = & - Z_c \left[\rho (2k_0 t^{-1} + 3k_1 t^{-2}) + k_2 \rho^2 (1 - 2t^{-2}) \right] + \\ & \frac{b\rho - b'\rho^2}{1 - b\rho + b'\rho^2} \end{aligned} \quad (18)$$

In the above equation H_0 is the enthalpy of the low-pressure gas at temperature T . Therefore, its variation with respect to temperature can be expressed as

$$H_0 = H^0 + \int_{T_0}^T C_p^* dT = H^0 + T_c \int_{t_0}^t C_p^* dt \quad (19)$$

where H^0 is the enthalpy of the gas under a very low pressure and at a standard temperature T_0 , and t_0 is the reduced temperature for the standard temperature.

Substituting equation (19) into equation (18) leads to the desired relation $H = f_1(\rho, t)$ as follows:

$$H = z_c RT_c t \rho (2K_0 t^{-1} + 3K_1 t^{-2}) - z_c RT_c t K_2 \rho^2 (1 - 2t^{-2}) + RT_c t \frac{(b\rho - b'\rho^2)}{(1 - b\rho + b'\rho^2)} + T_c \int_{t_0}^t C_p^* dt + H^0 \quad (20)$$

5. Entropy of a Non-ideal Gas: $S = f_2(\rho, t)$

Hirshfelder et al. have given detailed expressions for $\ln(f/p_c)$ and $(H-H_0)/RT$ without showing the detailed derivation. From these equations $(S-S_0)/R$ can be calculated and the desired S-function can be found. Instead of following the treatise given by them, a detailed derivation of the S-function will be given

One of Maxwell's relations is

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V \quad (21)$$

Therefore, under constant temperature, one has

$$dS_T = \left(\frac{\partial P}{\partial T}\right)_V dV \quad (22)$$

Since,

$$P = P_c \rho, \quad T = T_c t, \quad \text{and} \quad V = V_c / \rho,$$

the above equation can be rewritten as

$$\begin{aligned} dS &= - \frac{P_c V_c}{T_c} \left(\frac{\partial p}{\partial t}\right)_\rho \frac{d\rho}{\rho^2} = - R \frac{P_c V_c}{R T_c} \left(\frac{\partial p}{\partial t}\right)_\rho \frac{d\rho}{\rho^2} \\ &= - z_c R \left(\frac{\partial p}{\partial t}\right)_\rho \frac{d\rho}{\rho^2} \end{aligned} \quad (23)$$

For a hypothetical ideal gas, one has

$$dS^* = \left(\frac{\partial P}{\partial T} \right)_V \cdot dV = \frac{R}{V} \cdot dV = \frac{R}{V_c} \cdot V_c \cdot \frac{-d\rho}{\rho^2} = -R \cdot \frac{d\rho}{\rho^2} \quad (24)$$

Referring to Figure 7, we let state 1 represent a real gas at T, P, V and let state 2 represent a hypothetical ideal gas at the same temperature and volume as the real gas of state 1, and let state 3 represent a hypothetical ideal gas at critical pressure P_c and at the same temperature as states 1 and 2. Let S, S_2^* , and S_0' represent the entropy per mole of the gas under states 1, 2, and 3 respectively.

$S - S_2^*$ can be obtained by integrating $dS - dS^*$.

Thus,

$$\begin{aligned} S - S_2^* &= \int dS - \int dS^* \\ &= - \int_0^{\rho} \left[z_c R \left(\frac{\partial P}{\partial T} \right)_\rho \right] \frac{d\rho}{\rho^2} + \int_0^{\rho} R \cdot \rho \frac{d\rho}{\rho^2} \end{aligned}$$

Therefore,

$$\frac{S - S_2^*}{R} = \int_0^{\rho} \left[-z_c \left(\frac{\partial P}{\partial T} \right)_\rho + \rho \right] \frac{d\rho}{\rho^2} \quad (25)$$

Letting V_2^* and V_0' be the volume of the hypothetical ideal gas at state 2 and state 3 respectively, $S_2^* - S_0'$ can be expressed as

$$S_2^* - S_0' = R \ln \frac{V_2^*}{V_0'} \quad (26)$$

As has been described, the volume of state 2 is equal to that of state 1. Therefore,

$$S_2^* - S_0' = R \ln \frac{V}{V_0'} \quad (27)$$

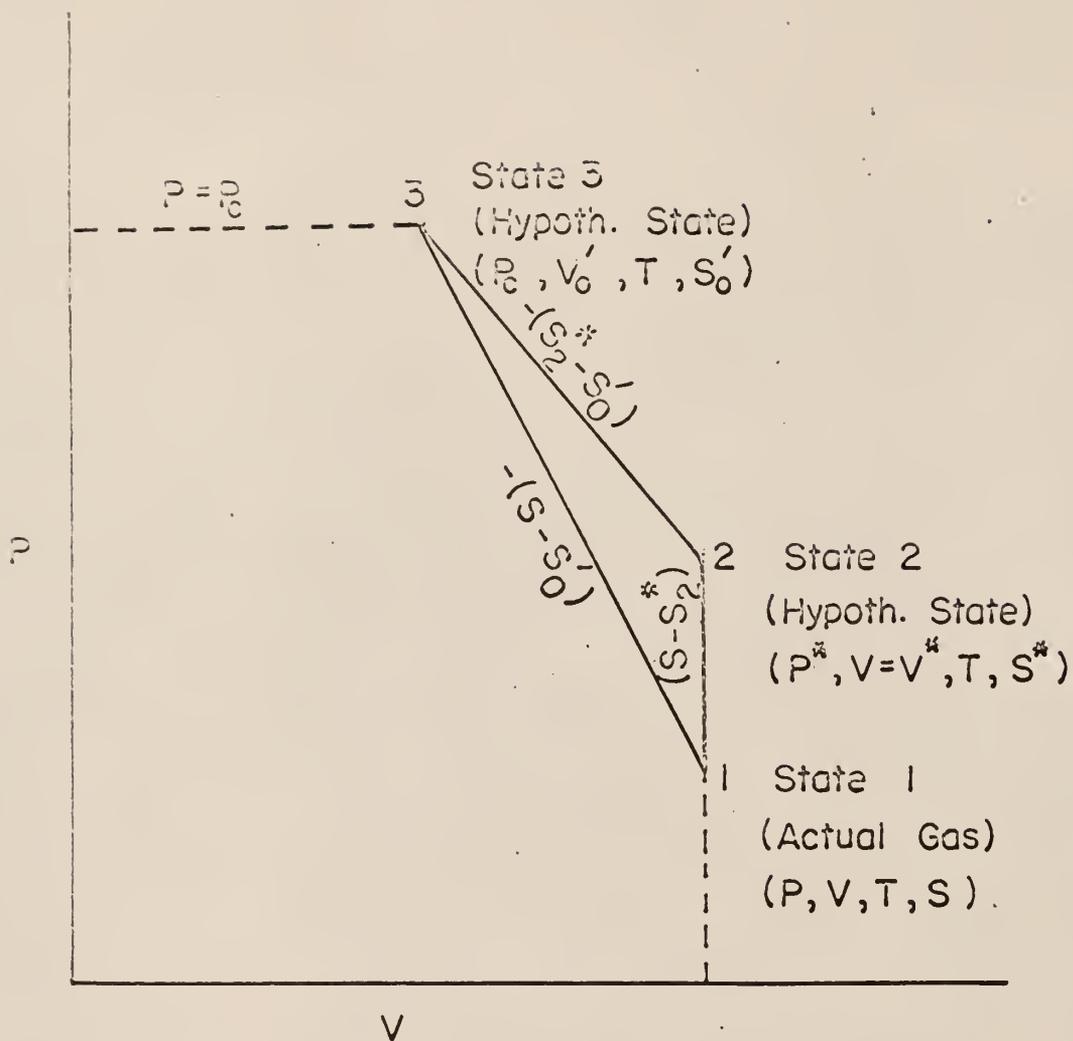


Fig. 7. Evaluation of S for a non-ideal gas.

Since according to the definition of V_o'

$$P_c \cdot V_o' = RT,$$

equation (27) can be written as

$$\frac{S_2^* - S_o'}{R} = \ln \frac{V}{\frac{RT}{P_c}} \quad (28)$$

Introducing the relations equations (11) into the above equation, one has

$$\begin{aligned} \frac{S_2^* - S_o'}{R} &= \ln \frac{P_c V_c \cdot (1/\rho)}{R T_c t} \\ &= \ln Z_c - \ln (\rho t) \end{aligned} \quad (29)$$

By subtracting equation (29) from equation (25), one has

$$\frac{S - S_o'}{R} = \int_0^\rho \left[-Z_c \left(\frac{\partial P}{\partial t} \right)_\rho + \rho \right] \frac{d\rho}{\rho^2} + \ln (\rho t) - \ln Z_c \quad (30)$$

This is the desired thermodynamic excess function for entropy. The desired S-function can be obtained by substituting the equation of state, equation (1) of this chapter into this equation.

$$\begin{aligned} \frac{S - S_o'}{R} &= -Z_c \left[-\frac{1}{2} k_2 \rho^2 + (k_1 \rho - \frac{1}{2} k_2 \rho^2) t^{-2} \right] - \ln (\rho t) \\ &+ \frac{1}{2} \ln(1 - b \rho + b' \rho^2) - k_3 \tan^{-1} k_3 - k_3 \tan^{-1}(k_4 \rho - k_3) + \ln Z_c \\ &= Z_c \left[-k_1 \rho t^{-2} + \frac{1}{2} k_2 \rho^2 (1 + t^{-2}) \right] - \ln(\rho t) \\ &+ \frac{1}{2} \ln(1 - b \rho + b' \rho^2) - k_3 \tan^{-1} k_3 - k_3 \tan^{-1}(k_4 \rho - k_3) + \ln Z_c \end{aligned} \quad (31)$$

Letting S_0 be the entropy of the gas at a hypothetical ideal gas state at the standard pressure P_0 (usually assumed at 1 atm), under the same temperature one has

$$S_0' = S_0 + R \ln (P_0/P_c). \quad (32)$$

Letting S^0 be the entropy of the gas at a hypothetical standard pressure P_0 and at a standard temperature T_0 , one has

$$S_0 - S^0 = \int_{T_0}^T \frac{C_p}{T} dT = \int_{t_0}^t \frac{C_p}{t} dt \quad (33)$$

where t and t_0 are reduced temperatures of T and T_0 respectively.

Introducing equations (32) and (33) into equation (31) and on rearranging, yields

$$S = R \left\{ Z_c \left[-k_1 \rho t^{-2} + \frac{1}{2} k_2 \rho^2 (1 + t^{-2}) \right] - \ln(\rho t) + \frac{1}{2} \ln(1 - b\rho + b'\rho^2) \right. \\ \left. - k_3 \tan^{-1} k_3 - k_3 \tan^{-1} (k_4 \rho - k_3) + \ln Z_c \right\} + S^0 + \int_{t_0}^t \frac{C_p dt}{t} + R \ln(P_0/P_c) \quad (34)$$

This is the desired equation

$$S = f_2(\rho, t)$$

CHAPTER 4. PERFORMANCE EQUATIONS, CONSTRAINT RELATIONS AND THEIR DERIVATIVES

A system analysis of a multistage gas compression system has been made and definitions of the state variables and decision variables presented in Chapter 2. Quantitative relations relating p , H and S to t and \mathcal{P} have been described in Chapter 3. With these relations available, the performance equations described in Chapter 2 can be formulated. In part A of this chapter quantitative relations for the performance equations and the constraint equations will be derived and in Part B first derivatives of these functions which will be used in the later optimization study will be given. In the present study, gas compression within region I only is considered. The procedure developed in this study can be easily extended to other regions.

PART A. PERFORMANCE EQUATIONS AND CONSTRAINT EQUATIONS

Figure 8 illustrates the mathematical model of a multistage gas compression system and summarizes the definitions of decision variables and state variables.

1. $x_1^n = T_1^n(\theta_1^n, \theta_4^n)$: Pressure at the n -th stage.

The pressure of a gas is related to its reduced temperature and reduced density by the generalized equation of state, equation (1) of Chapter 3. Since the pressure at the n -th stage can be related to $t_n' (= \theta_1^n)$ and $\rho_n' (= \theta_4^n)$, $t_n'' (= \theta_2^n)$ and $\rho_n'' (= \theta_5^n)$, and $t_n (= \theta_3^n)$ and $\rho_n (= \theta_6^n)$, respectively, the following equations can be written using the state space notation for the multistage process.

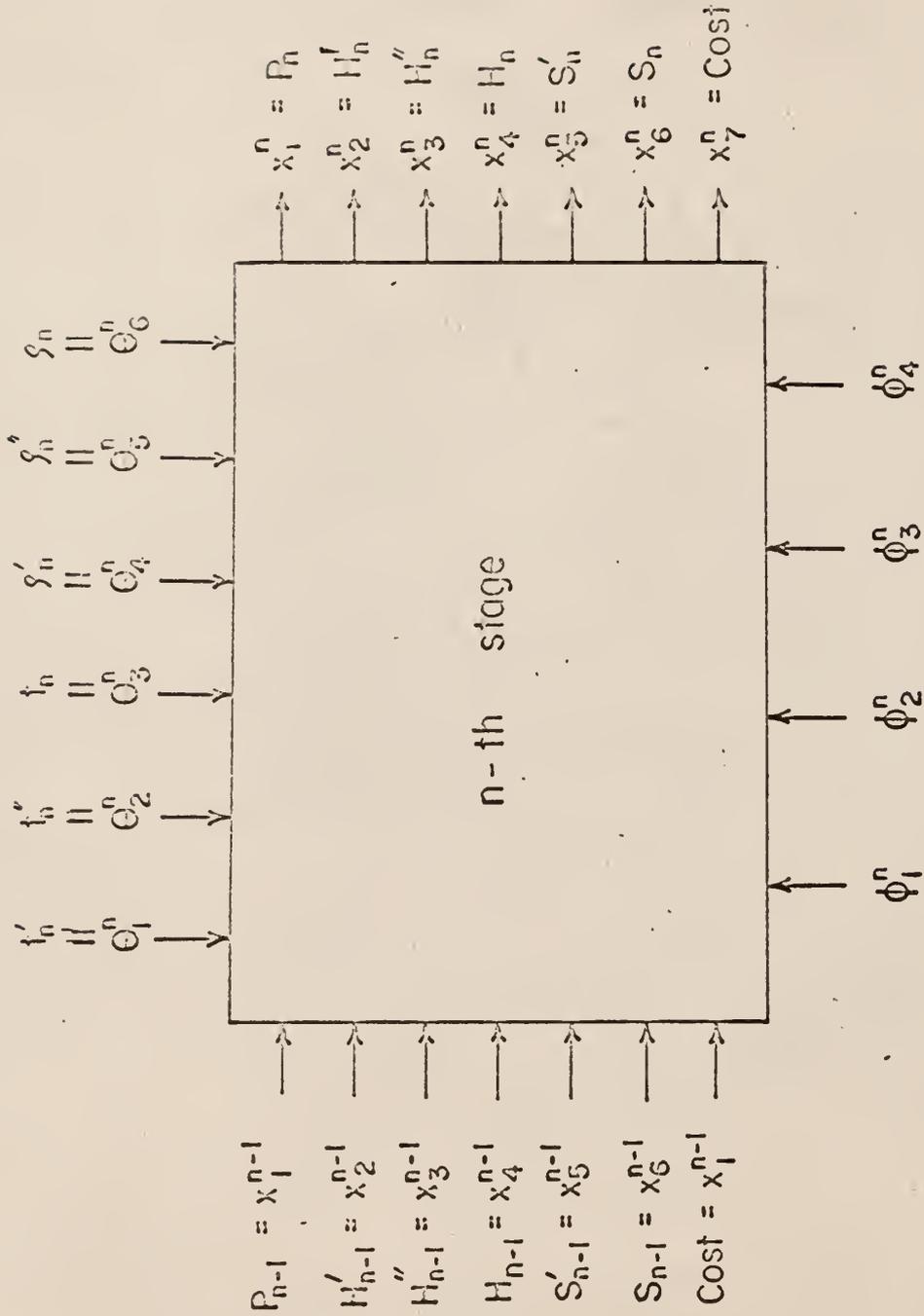


Fig. 8 . The decision and state variables at the n - th stage .

$$x_1^n = - [k_0 + k_1(\theta_1^n)^{-1}] (\theta_4^n)^2 + k_2 [-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^3 + \frac{(\theta_4^n \theta_1^n)}{z_c} / [1 - b(\theta_4^n) + b'(\theta_4^n)^2] \quad (1)$$

$$x_1^n = - [k_0 + k_1(\theta_2^n)^{-1}] (\theta_5^n)^2 + k_2 [-\theta_2^n + (\theta_2^n)^{-1}] (\theta_5^n)^3 + \frac{(\theta_5^n \theta_2^n)}{z_c} / [1 - b(\theta_5^n) + b'(\theta_5^n)^2] \quad (2)$$

$$x_1^n = - [k_0 + k_1(\theta_3^n)^{-1}] (\theta_6^n)^2 + k_2 [-\theta_3^n + (\theta_3^n)^{-1}] (\theta_6^n)^3 + \frac{(\theta_6^n \theta_3^n)}{z_c} / [1 - b(\theta_6^n) + b'(\theta_6^n)^2] \quad (3)$$

Equation (1) will be considered to be the performance equation for x_1^n . Equations obtained by equating equation (1) to equation (2) and by equating equation (1) to equation (3) will be considered as constraint relations. These constraint relations will be further described later.

2. $x_2^n = T_2^n (\theta_1^n, \theta_4^n)$: Enthalpy of the gas after the hypothetical reversible compression in the n-th stage.

The enthalpy, H, of a gas is related to its reduced temperature and reduced density by equation (20) of Chapter 3. Therefore, one can write

$$x_2^n = -z_c RT_c (2k_0) \theta_4^n - z_c RT_c (3k_1) (\theta_1^n)^{-1} (\theta_4^n) - z_c RT_c (k_2) (\theta_1^n) (\theta_4^n)^2 + z_c RT_c (2k_2) (\theta_1^n)^{-1} (\theta_4^n)^2 + RT_c (\theta_1^n) \frac{\{b(\theta_4^n) - b'(\theta_4^n)^2\}}{\{1 - b(\theta_4^n) + b'(\theta_4^n)^2\}} + \int_{t_0}^{\theta_1^n} C_p^* T_c d\theta_1^n + H^0 \quad (4)$$

where H^0 is the enthalpy per mole of the gas under hypothetical ideal state at the standard temperature T_0 .

3. $X_3^n = T_3^n (\theta_2^n, \theta_5^n)$: Enthalpy of the gas after actual compression in the n -th stage.

The performance equation for X_3^n can be obtained simply by replacing X_2^n , θ_1^n , and θ_4^n in equation (4) by X_3^n , θ_2^n and θ_5^n respectively. Thus we obtain

$$\begin{aligned}
 X_3^n = & -Z_c RT_c (2k_0) \theta_5^n - Z_c RT_c (3k_1) (\theta_2^n)^{-1} (\theta_5^n) - Z_c RT_c (k_2) (\theta_2^n) (\theta_5^n)^2 \\
 & + Z_c RT_c (2k_2) (\theta_2^n)^{-1} (\theta_5^n)^2 + RT_c (\theta_2^n) \frac{\{b(\theta_5^n) - b'(\theta_5^n)^2\}}{\{1 - b(\theta_5^n) + b'(\theta_5^n)^2\}} \\
 & + \int_{t_0}^{\theta_2^n} C_p^* T_c d\theta_2^n + H^0 \quad (5)
 \end{aligned}$$

4. $X_4^n = T_4^n (\theta_3^n, \theta_6^n)$: Enthalpy of the gas after actual compression and cooling in the n -th stage.

The performance equation for X_4^n can be obtained simply by replacing X_2^n , θ_1^n , and θ_4^n in equation (4) by X_4^n , θ_3^n and θ_6^n respectively. Thus we obtain

$$\begin{aligned}
 X_4^n = & -Z_c RT_c (2k_0) \theta_6^n - Z_c RT_c (3k_1) (\theta_3^n)^{-1} (\theta_6^n) - Z_c RT_c (k_2) (\theta_3^n) (\theta_6^n)^2 \\
 & + Z_c RT_c (2k_2) (\theta_3^n)^{-1} (\theta_6^n)^2 + RT_c (\theta_3^n) \frac{\{b(\theta_6^n) - b'(\theta_6^n)^2\}}{\{1 - b(\theta_6^n) + b'(\theta_6^n)^2\}} \\
 & + \int_{t_0}^{\theta_3^n} C_p^* T_c d\theta_3^n + H^0 \quad (6)
 \end{aligned}$$

5. $X_5^n = T_5^n (\theta_1^n, \theta_4^n)$: Entropy of the gas after the hypothetical reversible compression in the n -th stage.

The entropy, S , of a gas is related to its reduced temperature and reduced density through equation (34) of Chapter 3. Therefore one has

$$\begin{aligned}
 x_5^n &= (Z_c R)(-k_1)(\theta_1^n)^{-2} (\theta_4^n) + (Z_c R)\left(\frac{1}{2} k_2\right) \left\{ 1 + (\theta_1^n)^{-2} \right\} (\theta_4^n)^2 \\
 &- R \ln \left\{ (\theta_1^n)(\theta_4^n) \right\} + \frac{1}{2} R \ln \left\{ 1 - b(\theta_4^n) + b'(\theta_4^n)^2 \right\} - R k_3 \tan^{-1} k_3 \\
 &- R k_3 \tan^{-1} \left\{ k_4(\theta_4^n) - k_3 \right\} + R \ln Z_c + R \ln (P_o/P_c) + S^o + \\
 &\int_{t_o}^{\theta_1^n} \frac{C_p d\theta_1^n}{\theta_1^n} \tag{7}
 \end{aligned}$$

where S^o is the entropy per mole of the gas under hypothetical ideal state at 1 atm and standard temperature T_o .

6. $x_6^n = T_6^n (\theta_3^n, \theta_6^n)$: Entropy of the gas after actual compression and cooling in the n -th stage.

The performance equation for x_6^n can be obtained simply by replacing x_5^n , θ_1^n , and θ_4^n in equation (7) with x_6^n , θ_3^n , and θ_6^n respectively.

Thus one has

$$\begin{aligned}
 x_6^n &= (Z_c R)(-k_1)(\theta_3^n)^{-2} (\theta_6^n) + (Z_c R)\left(\frac{1}{2} k_2\right) \left\{ 1 + (\theta_3^n)^{-2} \right\} (\theta_6^n)^2 \\
 &- R \ln \left\{ (\theta_3^n)(\theta_6^n) \right\} + \frac{1}{2} R \ln \left\{ 1 - b(\theta_6^n) + b'(\theta_6^n)^2 \right\} - R k_3 \tan^{-1} k_3 \\
 &- R k_3 \tan^{-1} \left\{ k_4(\theta_6^n) - k_3 \right\} + R \ln Z_c + R \ln (P_o/P_c) + S^o \\
 &+ \int_{t_o}^{\theta_3^n} \frac{C_p d\theta_3^n}{\theta_3^n} \tag{8}
 \end{aligned}$$

7. $x_7^n = T_7^n(\theta_2^n, \theta_3^n, \theta_6^n, \theta_7^n, x_4^{n-1}, x_7^{n-1})$: The cumulative cost for compressing a mole of gas up to and including the n-th stage.

By substituting values and H and H'' from equations (20) of Chapter 3 into equation (23) of Chapter 2, one has

$$\begin{aligned}
 x_7^n = & x_7^{n-1} + C_c [T_3^n(\theta_2^n, \theta_5^n) - x_4^{n-1}] + \psi_1 C_{HP} [T_3^n(\theta_2^n, \theta_5^n) \\
 & - x_4^{n-1}] + \frac{\psi_2 \cdot C_H}{U \cdot T_c} \frac{[T_3^n(\theta_2^n, \theta_5^n) - T_4^n(\theta_3^n, \theta_6^n)]}{[\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]} \ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i} \\
 & + \frac{C_w}{(C_p)_w T_c} \frac{[T_3^n(\theta_2^n, \theta_5^n) - T_4^n(\theta_3^n, \theta_6^n)]}{[(t_w)_o - (t_w)_i]} \quad (9)
 \end{aligned}$$

8. $\phi_1^n = \phi_1^n(\theta_1^n, \theta_2^n, \theta_4^n, \theta_6^n) = 0$, and

$$\phi_2^n = \phi_2^n(\theta_1^n, \theta_3^n, \theta_4^n, \theta_6^n) = 0$$

It has been described that the n-th stage pressure can be calculated by knowing t_n' and p_n' in equation (1), t_n'' and p_n'' in equation (2), t_n and p_n in equation (3) respectively. Therefore, these quantities are related through two constraint equations

$$\phi_1^n = T_1^n(\theta_1^n, \theta_4^n) - T_1^n(\theta_2^n, \theta_5^n) = 0 \quad (10)$$

$$\phi_2^n = T_1^n(\theta_1^n, \theta_4^n) - T_1^n(\theta_3^n, \theta_6^n) = 0 \quad (11)$$

By substituting equations (1), (2), and (3) into the above equations, one obtains

$$\begin{aligned}
 \phi_1^n &= - [k_0 + k_1(\theta_1^n)^{-1}] (\theta_4^n)^2 + k_2[-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^3 \\
 &\quad + \left(\frac{\theta_4^n \theta_1^n}{z_c}\right) / [1 - b(\theta_4^n) + b'(\theta_4^n)^2] + [k_c + k_1(\theta_2^n)^{-1}] (\theta_5^n)^2 \\
 &\quad - k_2[-\theta_2^n + (\theta_2^n)^{-1}] (\theta_5^n)^3 - \left(\frac{\theta_5^n \theta_1^n}{z_c}\right) / [1 - b(\theta_5^n) + b'(\theta_5^n)^2] \\
 &= 0 \tag{12}
 \end{aligned}$$

$$\begin{aligned}
 \phi_2^n &= - [k_0 + k_1(\theta_1^n)^{-1}] (\theta_4^n)^2 + k_2[-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^3 \\
 &\quad + \left(\frac{\theta_4^n \theta_1^n}{z_c}\right) / [1 - b(\theta_4^n) + b'(\theta_4^n)^2] - [k_0 + k_1(\theta_3^n)^{-1}] (\theta_6^n)^2 \\
 &\quad + k_2[-\theta_3^n + (\theta_3^n)^{-1}] (\theta_6^n)^3 + \left(\frac{\theta_6^n \theta_3^n}{z_c}\right) / [1 - b(\theta_6^n) + b'(\theta_6^n)^2] \\
 &= 0 \tag{13}
 \end{aligned}$$

9. $\phi_3^n = \phi_3^n(\theta_1^n, \theta_4^n, x_6^{n-1}) = 0$: The constraint equation due to

$$s_n = s_{n-1}$$

Referring to equation (19) of Chapter 2, one can note that

$$\phi_3^n = x_5^n (\theta_1^n, \theta_4^n) - x_6^{n-1} = 0 \quad (14)$$

By substituting equation (7) into the above equation, we obtain

$$\begin{aligned} \phi_3^n &= (Z_c R)(-k_1)(\theta_1^n)^{-2} (\theta_4^n) + (Z_c R)\left(\frac{1}{2} k_2\right) [1 + (\theta_1^n)^{-2}] (\theta_4^n)^2 \\ &\quad - R \ln \{ (\theta_1^n)(\theta_4^n) \} + \frac{1}{2} R \ln \{ 1 - b(\theta_4^n) + b'(\theta_4^n)^2 \} - R k_3 \tan^{-1} k_3 \\ &\quad - R k_3 \tan^{-1} \{ k_4(\theta_4^n) - k_3 \} + R \ln Z_c + R \ln (P_o/P_c) + S^o \\ &\quad + \int_{t_o}^{\theta_1^n} \frac{C_p^* d\theta_1^n}{\theta_1^n} - x_6^{n-1} = 0 \end{aligned} \quad (15)$$

10. $\phi_4^n = \phi_4^n(\theta_1^n, \theta_2^n, \theta_4^n, \theta_5^n, x_4^{n-1}) = 0$: The constraint equation for the compressor efficiency.

Referring to equation (22) of Chapter 2, one can note that

$$\phi_4^n = [T_3^n(\theta_2^n, \theta_5^n) - x_4^{n-1}] - \frac{1}{\gamma} [T_2^n(\theta_1^n, \theta_4^n) - x_4^{n-1}] = 0 \quad (16)$$

By substituting equations (4) and (5) into the above equation,

$$\begin{aligned}
\phi_4^n = & -Z_c RT_c (2k_0) \theta_5^n - Z_c RT_c (3k_1) (\theta_2^n)^{-1} (\theta_5^n) - Z_c RT_c (k_2) (\theta_2^n) (\theta_5^n)^2 \\
& + Z_c RT_c (2k_2) (\theta_2^n)^{-1} (\theta_5^n)^2 + RT_c (\theta_2^n) \frac{\{b(\theta_5^n) - b'(\theta_5^n)^2\}}{\{1 - b(\theta_5^n) + b'(\theta_5^n)^2\}} \\
& + \int_{t_0}^{\theta_2^n} C_p^* T_c d\theta_2^n + H^0 - 1.2 \left[-Z_c RT_c (2k_0) \theta_4^n \right. \\
& - Z_c RT_c (3k_1) (\theta_1^n)^{-1} (\theta_4^n) - Z_c RT_c (k_2) (\theta_1^n) (\theta_4^n)^2 \\
& + Z_c RT_c (2k_2) (\theta_1^n)^{-1} (\theta_4^n)^2 + RT_c (\theta_1^n) \frac{\{b(\theta_4^n) - b'(\theta_4^n)^2\}}{\{1 - b(\theta_4^n) + b'(\theta_4^n)^2\}} \\
& \left. + \int_{t_0}^{\theta_1^n} C_p^* T_c d\theta_1^n + H^0 \right] + 0.2 X_4^{n-1} = 0 \tag{17}
\end{aligned}$$

PART B. THE FIRST DERIVATIVES OF THE STATE VARIABLES
AND THE CONSTRAINT FUNCTIONS

Table 3 shows the check list for the derivatives which will be used in the optimization study. These derivatives are obtained by differentiating the performance equations and constraint functions developed in Part A. The results of the differentiations are summarized as follows:

1. Derivatives of x_1^n with respect to θ_1^n , θ_2^n , θ_3^n , θ_4^n , θ_5^n and θ_6^n

Table 3. Check list for the first derivatives of the state variables and the constraint functions.

	x_1^n	x_2^n	x_3^n	x_4^n	x_5^n	x_6^n	x_7^n	ϕ_1^n	ϕ_2^n	ϕ_3^n	ϕ_4^n	Derivatives of Hamiltonian Function
θ_1^n	X	X			X			X	X	X	X	$\frac{\partial H^n}{\partial \theta_1^n} = \beta_1^n \frac{\partial x_1^n}{\partial \theta_1^n} + \beta_2^n \frac{\partial x_2^n}{\partial \theta_1^n} + \beta_5^n \frac{\partial x_5^n}{\partial \theta_1^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_1^n} + \lambda_1^n \frac{\partial \phi_1^n}{\partial \theta_1^n} + \lambda_2^n \frac{\partial \phi_2^n}{\partial \theta_1^n} + \lambda_3^n \frac{\partial \phi_3^n}{\partial \theta_1^n} + \lambda_4^n \frac{\partial \phi_4^n}{\partial \theta_1^n}$
θ_2^n	(X)		X				X	X			X	$\frac{\partial H^n}{\partial \theta_2^n} = \beta_3^n \frac{\partial x_3^n}{\partial \theta_2^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_2^n} + \lambda_1^n \frac{\partial \phi_1^n}{\partial \theta_2^n} + \lambda_4^n \frac{\partial \phi_4^n}{\partial \theta_2^n}$
θ_3^n	(X)			X		X			X			$\frac{\partial H^n}{\partial \theta_3^n} = \beta_4^n \frac{\partial x_4^n}{\partial \theta_3^n} + \beta_6^n \frac{\partial x_6^n}{\partial \theta_3^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_3^n} + \lambda_2^n \frac{\partial \phi_2^n}{\partial \theta_3^n}$
θ_4^n	X	X			X			X	X	X	X	$\frac{\partial H^n}{\partial \theta_4^n} = \beta_1^n \frac{\partial x_1^n}{\partial \theta_4^n} + \beta_2^n \frac{\partial x_2^n}{\partial \theta_4^n} + \beta_5^n \frac{\partial x_5^n}{\partial \theta_4^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_4^n} + \lambda_1^n \frac{\partial \phi_1^n}{\partial \theta_4^n} + \lambda_2^n \frac{\partial \phi_2^n}{\partial \theta_4^n} + \lambda_3^n \frac{\partial \phi_3^n}{\partial \theta_4^n} + \lambda_4^n \frac{\partial \phi_4^n}{\partial \theta_4^n}$
θ_5^n	(X)		X				X	X			X	$\frac{\partial H^n}{\partial \theta_5^n} = \beta_3^n \frac{\partial x_3^n}{\partial \theta_5^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_5^n} + \lambda_1^n \frac{\partial \phi_1^n}{\partial \theta_5^n} + \lambda_4^n \frac{\partial \phi_4^n}{\partial \theta_5^n}$
θ_6^n	(X)			X		X		X	X			$\frac{\partial H^n}{\partial \theta_6^n} = \beta_4^n \frac{\partial x_4^n}{\partial \theta_6^n} + \beta_6^n \frac{\partial x_6^n}{\partial \theta_6^n} + \beta_7^n \frac{\partial x_7^n}{\partial \theta_6^n} + \lambda_2^n \frac{\partial \phi_2^n}{\partial \theta_6^n}$
x_1^{n-1}												$\beta_1^{n-1} = 0$
x_2^{n-1}												$\beta_2^{n-1} = 0$
x_3^{n-1}												$\beta_3^{n-1} = 0$
x_4^{n-1}							X				X	$\beta_4^{n-1} = \beta_1^n \frac{\partial x_1^n}{\partial x_4^{n-1}} + \lambda_4^n \frac{\partial \phi_4^n}{\partial x_4^{n-1}}$
x_5^{n-1}												$\beta_5^{n-1} = 0$
x_6^{n-1}										X		$\beta_6^{n-1} = \lambda_3^n \frac{\partial \phi_3^n}{\partial x_6^{n-1}} = -\lambda_3^n$
x_7^{n-1}							X					$\beta_7^{n-1} = \beta_1^n \frac{\partial x_1^n}{\partial x_7^{n-1}} = 1$

$$\begin{aligned}
\frac{\partial x_1^n}{\partial \theta_1^n} &= k_1 (\theta_1^n)^{-2} (\theta_4^n)^2 + k_2 [-1 -1 (\theta_1^n)^{-2}] (\theta_4^n)^3 \\
&+ \frac{\theta_5^n}{z_c} / [1 - b(\theta_4^n) + b'(\theta_4^n)^2] = k_1 (\theta_1^n)^{-2} (\theta_4^n)^2 \\
&- k_2 (\theta_4^n)^3 - k_2 (\theta_1^n)^{-2} (\theta_4^n)^3 + \frac{(\theta_4^n)}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]} \quad (18)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial x_1^n}{\partial \theta_2^n} &= k_1 (\theta_2^n)^{-2} (\theta_5^n)^2 - k_2 (\theta_5^n)^3 - k_2 (\theta_2^n)^{-2} (\theta_5^n)^3 \\
&+ \frac{(\theta_5^n)}{z_c [1 - b(\theta_5^n) + b'(\theta_5^n)^2]} \quad (19)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial x_1^n}{\partial \theta_3^n} &= k_1 (\theta_3^n)^{-2} (\theta_6^n)^2 - k_2 (\theta_6^n)^3 - k_2 (\theta_3^n)^{-2} (\theta_6^n)^3 \\
&+ \frac{(\theta_6^n)}{z_c [1 - b(\theta_6^n) + b'(\theta_6^n)^2]} \quad (20)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial x_1^n}{\partial \theta_4^n} &= -2 [k_0 + k_1 (\theta_1^n)^{-1}] (\theta_4^n) + 3 k_2 [-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^2 \\
&+ \frac{\theta_1^n}{z_c} / [1 - b(\theta_4^n) + b'(\theta_4^n)^2] + \frac{\theta_5^n \theta_1^n}{z_c} \frac{(-1) [-b + 2b'(\theta_4^n)]}{[1 - b(\theta_4^n) + b'(\theta_4^n)^2]^2} \\
&= -2 [k_0 + k_1 (\theta_1^n)^{-1}] (\theta_4^n) + 3 k_2 [-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^2 \\
&+ \frac{[1 - b(\theta_4^n) + b'(\theta_4^n)^2] (\theta_1^n) - \theta_4^n \theta_1^n [-b + 2b'(\theta_4^n)]}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]^2} \quad (21)
\end{aligned}$$

$$\begin{aligned} \frac{\partial x_1^n}{\partial \theta_5^n} &= -2[k_0 + k_1(\theta_2^n)^{-1}] (\theta_5^n) + 3k_2[-\theta_2^n + (\theta_2^n)^{-1}] (\theta_5^n)^2 \\ &+ \frac{[1 - b(\theta_5^n) + b'(\theta_5^n)^2] (\theta_2^n) - \theta_5^n \theta_2^n [-b + 2b'(\theta_5^n)]}{z_c [1 - b(\theta_5^n) + b'(\theta_5^n)^2]^2} \end{aligned} \quad (22)$$

$$\begin{aligned} \frac{\partial x_1^n}{\partial \theta_6^n} &= -2[k_0 + k_1(\theta_3^n)^{-1}] (\theta_6^n) + 3k_2[-\theta_3^n + (\theta_3^n)^{-1}] (\theta_6^n)^2 \\ &+ \frac{[1 - b(\theta_6^n) + b'(\theta_6^n)^2] (\theta_3^n) - \theta_6^n \theta_3^n [-b + 2b'(\theta_6^n)]}{z_c [1 - b(\theta_6^n) + b'(\theta_6^n)^2]^2} \end{aligned} \quad (23)$$

2. Derivatives of x_2^n with respect to θ_1^n and θ_4^n

$$\begin{aligned} \frac{\partial x_2^n}{\partial \theta_1^n} &= + (z_c RT_c)(3k_1)(\theta_1^n)^{-2} (\theta_4^n) - (z_c RT_c)(k_2)(\theta_4^n)^2 \\ &- (z_c RT_c)(2k_2)(\theta_1^n)^{-2} (\theta_4^n)^2 + RT_c \frac{[b(\theta_4^n) - b'(\theta_4^n)^2]}{[1 - b(\theta_4^n) + b'(\theta_4^n)^2]} \\ &+ C_p^* T_c \end{aligned} \quad (24)$$

$$\begin{aligned} \frac{\partial x_2^n}{\partial \theta_4^n} &= - (z_c RT_c)(2k_0) - (z_c RT_c)(3k_1)(\theta_1^n)^{-1} - (z_c RT_c)(2k_2)(\theta_1^n)(\theta_4^n) \\ &+ (z_c RT_c)(4k_2)(\theta_1^n)^{-1} (\theta_4^n) + (RT_c)(\theta_1^n) \frac{[+b - 2b'(\theta_4^n)]}{[1 - b(\theta_4^n) + b'(\theta_4^n)^2]^2} \end{aligned} \quad (25)$$

3. Derivatives of x_3^n with respect to θ_2^n and θ_5^n

$$\begin{aligned} \frac{\partial x_2^n}{\partial \theta_2^n} &= + (Z_c RT_c)(3k_1)(\theta_2^n)^{-2} (\theta_5^n) - (Z_c RT_c)(k_2)(\theta_5^n)^2 \\ &- (Z_c RT_c)(2k_2)(\theta_2^n)^{-2} (\theta_5^n)^2 + RT_c \frac{[b(\theta_5^n) - b'(\theta_5^n)^2]}{[1-b(\theta_5^n) + b'(\theta_5^n)^2]} \\ &+ C_p^* T_c \end{aligned} \quad (26)$$

$$\begin{aligned} \frac{\partial x_2^n}{\partial \theta_5^n} &= - (Z_c RT_c)(2k_0) - (Z_c RT_c)(3k_1)(\theta_2^n)^{-1} - (Z_c RT_c)(2k_2)(\theta_2^n)(\theta_5^n) \\ &+ (Z_c RT_c)(4k_2)(\theta_2^n)^{-1} (\theta_5^n) + (RT_c)(\theta_2^n) \frac{[+b - 2b'(\theta_5^n)]}{[1-b(\theta_5^n) + b'(\theta_5^n)^2]^2} \end{aligned} \quad (27)$$

4. Derivatives of x_4^n with respect to θ_3^n and θ_6^n

$$\begin{aligned} \frac{\partial x_4^n}{\partial \theta_3^n} &= + (Z_c RT_c)(3k_1)(\theta_1^n)^{-2} (\theta_6^n) - (Z_c RT_c)(k_2)(\theta_6^n)^2 \\ &- (Z_c RT_c)(2k_2)(\theta_3^n)^{-2} (\theta_6^n)^2 + RT_c \frac{[b(\theta_6^n) - b'(\theta_6^n)^2]}{[1-b(\theta_6^n) + b'(\theta_6^n)^2]} + C_p^* T_c \end{aligned} \quad (28)$$

$$\begin{aligned} \frac{\partial x_4^n}{\partial \theta_6^n} &= -(Z_c R T_c)(2k_0) - (Z_c R T_c)(3k_1)(\theta_3^n)^{-1} - (Z_c R T_c)(2k_2)(\theta_3^n)(\theta_6^n) \\ &+ (Z_c R T_c)(4k_2)(\theta_3^n)^{-1} (\theta_6^n) + (R T_c)(\theta_3^n) \frac{\{+b - 2b'(\theta_6^n)\}}{\{1 - b(\theta_6^n) + b'(\theta_6^n)^2\}^2} \quad (29) \end{aligned}$$

5. Derivatives of x_5^n with respect to θ_1^n and θ_4^n .

$$\begin{aligned} \frac{\partial x_5^n}{\partial \theta_1^n} &= (Z_c R)(2k_1)(\theta_1^n)^{-3} (\theta_4^n) + (Z_c R)\left(\frac{1}{2} k_2\right) \{ -2(\theta_1^n)^{-3} \} (\theta_4^n)^2 \\ &- R \frac{\theta_5^n}{(\theta_1^n)(\theta_4^n)} + \frac{C_p}{\theta_1^n} = (Z_c R)(2k_1)(\theta_1^n)^{-3} (\theta_4^n) - (Z_c R) k_2 (\theta_1^n)^{-3} (\theta_4^n)^2 \\ &- R(\theta_1^n)^{-1} + C_p(\theta_1^n)^{-1} \quad (30) \end{aligned}$$

$$\begin{aligned} \frac{\partial x_5^n}{\partial \theta_4^n} &= (Z_c R)(-k_1)(\theta_1^n)^{-2} + (Z_c R)(k_2) \{ 1 + (\theta_1^n)^{-2} \} (\theta_4^n) - R(\theta_4^n)^{-1} \\ &+ \frac{1}{2} R \frac{-b + 2b'(\theta_4^n)}{\{1 - b(\theta_4^n) + b'(\theta_4^n)^2\}} - R k_3 \frac{k_4}{1 + [k_4(\theta_4^n) - k_3]^2} \quad (31) \end{aligned}$$

6. Derivatives of x_6^n with respect to θ_3^n and θ_6^n .

$$\begin{aligned} \frac{\partial x_6^n}{\partial \theta_3^n} &= (Z_c R)(2k_1)(\theta_3^n)^{-3} (\theta_6^n) + (Z_c R)\left(\frac{1}{2} k_2\right) \{ -2(\theta_3^n)^{-3} \} (\theta_6^n)^2 \\ &- R \frac{\theta_5^n}{(\theta_3^n)(\theta_6^n)} + \frac{C_p}{\theta_3^n} = (Z_c R)(2k_1)(\theta_3^n)^{-3} (\theta_6^n) \\ &- (Z_c R) k_2 (\theta_3^n)^{-3} (\theta_6^n)^2 - R(\theta_3^n)^{-1} + C_p(\theta_3^n)^{-1} \quad (32) \end{aligned}$$

$$\frac{\partial x_6^n}{\partial \theta_6^n} = (Z_c R)(-k_1)(\theta_3^n)^{-2} + (Z_c R)(k_2) \{ 1 + (\theta_3^n)^{-2} \} (\theta_6^n) - R(\theta_6^n)^{-1} \\ + \frac{1}{2} R \frac{\{-b + 2b'(\theta_6^n)\}}{\{1 - b(\theta_6^n) + b'(\theta_6^n)^2\}} - R k_3 \frac{k_4}{1 + [k_4(\theta_6^n) - k_3]^2} \quad (33)$$

7. Derivatives of x_7^n with respect to θ_2^n , θ_3^n , θ_5^n , θ_6^n , x_4^{n-1} , x_7^{n-1}

$$\frac{\partial x_7^n}{\partial \theta_2^n} = \frac{\partial x_3^n}{\partial \theta_2^n} \left\{ C_e + \psi_1 C_{HP} + \frac{C_w}{(C_p)_w T_c} \frac{1}{(t_w)_o - (t_w)_i} \right. \\ \left. + \frac{\psi_2 C_H}{UT_c} \frac{\ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i}}{[\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]} \right\} \\ + \frac{\psi_2 C_H}{UT_c} \frac{(x_3^n - x_4^n) \{ [\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i] \} - \left[\ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i} \right] [\theta_2^n - (t_w)_o]}{\{ [\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i] \}^2 [\theta_2^n - (t_w)_o]} \quad (34)$$

$$\frac{\partial x_7^n}{\partial \theta_3^n} = - \left\{ \frac{\psi_2 C_H}{UT_c} \frac{\ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i}}{[\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]} \right. \\ \left. + \frac{C_w}{(C_p)_w T_c} \frac{1}{(t_w)_o - (t_w)_i} \right\} \left(\frac{\partial x_4^n}{\partial \theta_3^n} \right) - \frac{\psi_2 C_H}{UT_c} (x_3^n - x_4^n) \cdot \\ \frac{[\theta_3^n - (t_w)_i] \ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i} + [\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]}{\{ [\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i] \}^2 [\theta_3^n - (t_w)_i]} \quad (35)$$

$$\frac{\partial x_7^n}{\partial \theta_5^n} = \left(\frac{\partial x_3^n}{\partial \theta_5^n} \right) \left[c_e + \psi_1 c_{HP} + \frac{c_w}{(c_p)_w T_c} \frac{1}{(t_w)_o - (t_w)_i} \right. \\ \left. + \frac{\psi_2 c_H}{UT_c} \cdot \frac{\ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i}}{[\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]} \right] \quad (36)$$

$$\frac{\partial x_7^n}{\partial \theta_6^n} = - \left(\frac{\partial x_4^n}{\partial \theta_6^n} \right) \left[\frac{\psi_2 c_H}{UT_c} \frac{\ln \frac{\theta_2^n - (t_w)_o}{\theta_3^n - (t_w)_i}}{[\theta_2^n - (t_w)_o] - [\theta_3^n - (t_w)_i]} + \frac{c_w}{(c_p)_w T_c} \frac{1}{(t_w)_o - (t_w)_i} \right] \quad (37)$$

$$\frac{\partial x_7^n}{\partial x_4^{n-1}} = - [c_e + \psi_1 c_{HP}] \quad (38)$$

$$\frac{\partial x_7^n}{\partial x_7^{n-1}} = 1 \quad (39)$$

8. Derivatives of ϕ_1^n with respect to θ_1^n , θ_2^n , θ_4^n , and θ_5^n

$$\frac{\partial \phi_1^n}{\partial \theta_1^n} = k_1 (\theta_1^n)^{-2} (\theta_4^n)^2 - k_2 (\theta_4^n)^3 - k_2 (\theta_1^n)^{-2} (\theta_4^n)^3 \\ + \frac{(\theta_4^n)}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]} \quad (40)$$

$$\frac{\partial \phi_1^n}{\partial \theta_2^n} = k_1 (\theta_2^n)^{-2} (\theta_5^n)^2 - k_2 (\theta_5^n)^3 - k_2 (\theta_2^n)^{-2} (\theta_5^n)^3 \\ + \frac{(\theta_5^n)}{z_c [1 - b(\theta_5^n) + b'(\theta_5^n)^2]} \quad (41)$$

$$\frac{\partial \phi_1^n}{\partial \theta_4^n} = -2[k_0 + k_1(\theta_1^n)^{-1}] (\theta_4^n) + 3 k_2[-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^2$$

$$+ \frac{[1 - b(\theta_4^n) + b'(\theta_4^n)^2] (\theta_1^n) - \theta_4^n \theta_1^n [-b + 2b'(\theta_4^n)]}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]^2} \quad (42)$$

$$\frac{\partial \phi_1^n}{\partial \theta_5^n} = -2[k_0 + k_1(\theta_2^n)^{-1}] (\theta_5^n) + 3 k_2[-\theta_2^n + (\theta_2^n)^{-1}] (\theta_5^n)^2$$

$$+ \frac{[1 - b(\theta_5^n) + b'(\theta_5^n)^2] (\theta_2^n) - \theta_5^n \theta_2^n [-b + 2b'(\theta_5^n)]}{z_c [1 - b(\theta_5^n) + b'(\theta_5^n)^2]^2} \quad (43)$$

9. Derivatives of ϕ_2^n with respect to θ_1^n , θ_3^n , θ_4^n , and θ_6^n

$$\frac{\partial \phi_2^n}{\partial \theta_1^n} = k_1(\theta_1^n)^{-2} (\theta_4^n)^2 - k_2(\theta_4^n)^3 - k_2(\theta_1^n)^{-2} (\theta_4^n)^3$$

$$+ \frac{(\theta_4^n)}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]} \quad (44)$$

$$\frac{\partial \phi_2^n}{\partial \theta_3^n} = k_1(\theta_3^n)^{-2} (\theta_6^n)^2 - k_2(\theta_6^n)^3 - k_2(\theta_3^n)^{-2} (\theta_6^n)^3$$

$$+ \frac{(\theta_6^n)}{z_c [1 - b(\theta_6^n) + b'(\theta_6^n)^2]} \quad (45)$$

$$\frac{\partial \phi_2^n}{\partial \theta_4^n} = -2[k_0 + k_1(\theta_1^n)^{-1}] (\theta_4^n) + 3k_2[-\theta_1^n + (\theta_1^n)^{-1}] (\theta_4^n)^2$$

$$+ \frac{[1 - b(\theta_4^n) + b'(\theta_4^n)^2] (\theta_1^n) - \theta_4^n \theta_1^n [-b + 2b'(\theta_4^n)]}{z_c [1 - b(\theta_4^n) + b'(\theta_4^n)^2]^2} \quad (46)$$

$$\frac{\partial \phi_2^n}{\partial \theta_6^n} = -2[k_0 + k_1(\theta_1^n)^{-1}] (\theta_5^n) + 3k_2[-\theta_1^n + (\theta_1^n)^{-1}] (\theta_5^n)^2$$

$$+ \frac{[1 - b(\theta_5^n) + b'(\theta_5^n)^2] (\theta_1^n) - \theta_5^n \theta_1^n [-b + 2b'(\theta_5^n)]}{z_c [1 - b(\theta_5^n) + b'(\theta_5^n)^2]^2} \quad (47)$$

10. Derivatives of ϕ_3^n with respect to θ_1^n , θ_4^n , and x_6^{n-1}

$$\frac{\partial \phi_3^n}{\partial \theta_1^n} = (z_c R)(2k_1)(\theta_1^n)^{-3} (\theta_4^n) - (z_c R) k_2 (\theta_1^n)^{-3} (\theta_4^n)^2$$

$$- R(\theta_1^n)^{-1} + C_p(\theta_1^n)^{-1} \quad (48)$$

$$\frac{\partial \phi_3^n}{\partial \theta_4^n} = (z_c R)(-k_1)(\theta_1^n)^{-2} + (z_c R)(k_2) \{1 + (\theta_1^n)^{-2}\} (\theta_4^n) - R(\theta_4^n)^{-1}$$

$$+ \frac{1}{2} R \frac{-b + 2b'(\theta_4^n)}{1 - b(\theta_4^n) + b'(\theta_4^n)^2} - R k_3 \frac{k_4}{1 + [k_4(\theta_4^n) - k_3]^2} \quad (49)$$

$$\frac{\partial \phi_3^n}{\partial x_6^{n-1}} = -1 \quad (50)$$

11. Derivatives of ϕ_4^n with respect to θ_1^n , θ_2^n , θ_4^n , θ_5^n and \mathcal{I}_4^{n-1}

$$\begin{aligned} \frac{\partial \phi_4^n}{\partial \theta_1^n} = & - 1.2 \left[(Z_c RT_c)(3k_1)(\theta_1^n)^{-2} (\theta_4^n) - (Z_c RT_c)(k_2)(\theta_4^n)^2 \right. \\ & - (Z_c RT_c)(2k_2)(\theta_1^n)^{-2} (\theta_4^n)^2 + RT_c \frac{[b(\theta_4^n) - b'(\theta_4^n)^2]}{\{1 - b(\theta_4^n) + b'(\theta_4^n)^2\}} \\ & \left. + C_p^* T_c \right] \end{aligned} \quad (51)$$

$$\begin{aligned} \frac{\partial \phi_4^n}{\partial \theta_2^n} = & + (Z_c RT_c)(3k_1)(\theta_2^n)^{-2} (\theta_5^n) - (Z_c RT_c)(k_2)(\theta_5^n)^2 \\ & - (Z_c RT_c)(2k_2)(\theta_2^n)^{-2} (\theta_5^n)^2 + RT_c \frac{\{b(\theta_5^n) - b'(\theta_5^n)^2\}}{\{1 - b(\theta_5^n) + b'(\theta_5^n)^2\}} \\ & + C_p^* T_c \end{aligned} \quad (52)$$

$$\begin{aligned} \frac{\partial \phi_4^n}{\partial \theta_4^n} = & - 1.2 \left[- (Z_c RT_c)(2k_0) - (Z_c RT_c)(3k_1)(\theta_1^n)^{-1} \right. \\ & - (Z_c RT_c)(2k_2)(\theta_1^n)(\theta_4^n) + (Z_c RT_c)(4k_2)(\theta_1^n)^{-1} (\theta_4^n) \\ & \left. + (RT_c)(\theta_1^n) \frac{\{+ b - 2b'(\theta_4^n)\}}{\{1 - b(\theta_4^n) + b'(\theta_4^n)^2\}^2} \right] \end{aligned} \quad (53)$$

$$\frac{\partial \phi_4^n}{\partial \theta_5^n} = - (Z_c RT_c) (2k_0) - (Z_c RT_c) (3k_1) (\theta_2^n)^{-1} - (Z_c RT_c) (2k_2) (\theta_2^n) (\theta_5^n) \\ + (Z_c RT_c) (4k_2) (\theta_2^n)^{-1} (\theta_5^n) + (RT_c) (\theta_2^n) \frac{[+ b - 2b'(\theta_5^n)]}{[1 - b(\theta_5^n) + b'(\theta_5^n)^2]^2} \quad (54)$$

$$\frac{\partial \phi_4^n}{\partial x_4^{n-1}} = 0.2 \quad (55)$$

CHAPTER 5. OPTIMIZATION STUDY OF A MULTISTAGE
GAS COMPRESSION SYSTEM

1. INTRODUCTION

A system analysis of a multistage gas compression system has been made and the operating variables have been defined in Chapter 2. In Chapter 3, the reduced pressure of a gas, the entropy and the enthalpy of the gas per mole have been related to the reduced gas temperature and the reduced gas density. In Chapter 4, state space notation has been introduced and the quantitative relations among the operating variables have been summarized. Figure 5 shows a mathematical model of the 3-stage gas compression system. The functional relations among the operating variables as summarized in Chapter 4 conform to the conditional form of a discrete analog the maximum principle as

$$x_i^n = T_i^n(\theta_1^n, \theta_2^n, \dots, \theta_t^n, x_1^{n-1}, \dots, x_s^{n-1}) \quad (1)$$

where t and s are respectively the number of decision variables in the n -th stage and the number of state variables in the $(n-1)$ th stage.

It will be assumed that the following conditions are given in an optimization problem:

1. Gas temperature and gas pressure at the inlet.
2. Gas temperature and gas pressure at the discharge from the last stage. Referring to Fig. 3, it can be noted that the gas entering the first stage is the gas discharged from the hypothetical zero-th stage and, therefore, the reduced

pressure, x_1^0 , the enthalpy of the gas per mole, x_4^0 , the entropy of the gas per mole, x_6^0 at the inlet condition are functions of the reduced temperature θ_3^0 and the reduced density θ_6^n of the gas discharged from the zero-th stage. Knowing the gas temperature and gas pressure at the inlet, one can find the reduced temperature θ_3^0 and reduced pressure x_1^0 . Knowing θ_3^0 and x_1^0 , can find θ_6^0 , and consequently x_4^0 and x_6^0 . x_7^0 is assumed to be zero. Therefore, all of the θ_3^0 , θ_6^0 , x_1^0 , x_4^0 , x_6^0 , and x_3^0 are known values in the present gas compression problem.

Excluding the hypothetical zero-th stage from consideration (because the feed condition is fixed), and considering a three-stage gas compression system, the following operating variables can be identified.

1. There are six decision variables in each stage which are denoted as θ_i^n ($i = 1, \dots, 6$). Therefore, there are $6 \times N = 6 \times 3 = 18$ decision variables in the whole system.
2. There are seven state variables in each stage which are denoted as x_j^n ($j = 1, \dots, 7$). Therefore, there are $7 \times N = 7 \times 3 = 21$ state variables in the whole system.

Among these operating variables, there are the following relations:

1. All the state variables x_j^n 's can be expressed as functions of θ^n and x_k^{n-1} by equations of the form of equation (1). There are $7 \times N = 7 \times 3 = 21$ relations.

2. In each stage, there exist four constraint equations:

$$\phi_i^n = 0, \quad i = 1, 2, 3, 4.$$

There are $4 \times N = 4 \times 3 = 12$ relations.

3. The temperature and pressure of the discharge gas are given as stated above. Therefore, there are 2 additional relations.

From the above analysis, it is seen that the number of independent variables in a 3-stage gas compression system is

$$(6N + 7N) - (7N + 4N + 2) = (2N - 2) = 2(N-1) = 4$$

In a general N-stage system, the number of independent variables is given as $2(N-1)$.

For the present study of a three-stage gas compression system, truly independent variables are chosen as

$$\theta_1^1, \theta_3^1, \theta_1^2 \text{ and } \theta_3^2.$$

When a set of values are assigned to these four decision variables, it is possible to determine all the remaining operating variables shown in Figure 3, and the gas compression cost x_7^3 can also be determined.

An optimization problem for a multistage (say N-stage) gas compression can be stated as follows:

In compressing a gas (say CO_2 gas) by a N-stage gas compression system from a given initial condition (i.e. θ_3^0 and x_1^0 are given) to a given discharge condition (i.e. θ_3^N and x_1^N are given), find a set of values for $\{\theta_1^1, \theta_3^1, \theta_1^2, \theta_3^2, \dots, \theta_1^{N-1}, \theta_3^{N-1}\}$ which will give

the minimum value for the objective function x_7^N . A three-stage system is treated in this study.

In the following sections, the following problems will be specifically considered.

1. Given a set of values for the independent variables, $\{\theta_1^1, \theta_3^1, \theta_1^2, \theta_3^2\}$, determine the remaining operating variables. This problem will be described in section 3.
2. Establish the algorithm for finding the optimum set of $\{\theta_1^1, \theta_3^1, \theta_1^2, \theta_3^2\}$. This problem is described in section 2.
3. Establish an iterative numerical computational scheme for finding the optimum set of independent variables. This problem is described in section 4.

II. FINDING THE OPTIMAL POLICY OF A MULTISTAGE MULTIDECISION PROCESS WITH EQUALITY CONSTRAINTS IN EACH STAGE --GENERAL DISCUSSION

In this section, we shall discuss an algorithm for finding the optimal policy for a multistage (say 3-stage) process having six decision variables, seven state variables, and four equality constraints in each stage and a state variable at the last stage being fixed. The objective function is assumed to be expressible in the following form

$$S = \sum_{i=1}^7 C_i^N \cdot x_i^N \quad (2)$$

The algorithm obtained in this section can easily be generalized to any number of stages, any number of decision variables, any number of state variables and any number of equality constraints.

The general functional relations are summarized as

1. Performance equations

$$x_i^n = T_i^n (x_1^{n-1}, \dots, x_7^{n-1}; \theta_1^n, \dots, \theta_6^n) \quad (3)$$

for $i = 1, 2, \dots, 7,$

and $n = 1, 2, 3.$

2. Constraint relations

$$\phi_j^n = \phi_j^n (x_1^{n-1}, \dots, x_7^{n-1}, \theta_1^n, \dots, \theta_6^n) = 0 \quad (4)$$

for $j = 1, 2, 3, 4$

and $n = 1, 2, 3.$

3. x_1^3 and θ_3^3 are given values.

4. x_i^0 for $i = 1, 2, \dots, 7$ are known values.

With these assumptions, there are four independent variables which are chosen to be $\theta_1^1, \theta_3^1, \theta_1^2$ and θ_3^2 .

According to the classical differential calculus, the necessary condition for an extremum of the objective function, when all the independent variables are unbounded, is that the total differential of the objective function be zero, i.e. $dS = 0$. It will be shown that the exact differential of the objective function can be expressed in terms of the differentials of the independent variables as

$$dS = [A] d\theta_1^1 + [B] d\theta_3^1 + [C] d\theta_1^2 + [D] d\theta_3^2 \quad (5)$$

by eliminating the differentials of all the dependent variables utilizing equations (3) and (4). Since the above equation contains only differentials of independent variables which can be arbitrarily varied, all the bracketed terms in equation (5) should be zero.

There are two ways by which dS can be expressed in the form of equation (5). They are: (i) direct substitution followed by differentiation, and (ii) differentiation followed by substitution. In the former approach, the performance equations as represented by equation (3) and the constraint equations as represented by equation (4) are successively substituted into the objective function, equation (2), and the resulting equation is then differentiated. In the latter approach, equations (2), (3), and (4) are differentiated and the differential forms of equations (3) and (4) are successively substituted into the differential form of equation (2). Such successive substitutions become increasingly difficult as the number of stages, state variables and decision variables and equality constraints increase. It will be shown that when the adjoint variables, Lagrange multipliers and Hamiltonian functions are introduced, the substitution procedure can be simplified. It will further be shown that the essential features of the algorithm to be developed can be arrived at by comparing the two approaches.

1. Direct substitution followed by differentiation.

Equations (3) and (4) can be written in expanded forms as

$$x_i^1 = T_i^1 \{x^0, \theta^1\} \quad \text{for } i = 1, \dots, 7 \quad (6-a)$$

$$x_i^2 = T_i^2 \{x^1, \theta^2\} \quad \text{"} \quad (6-b)$$

$$x_i^3 = T_i^3 \{x^2, \theta^3\} \quad \text{"} \quad (6-c)$$

$$\phi_i^1 = \phi_i^1 \{x^0, \theta^1\} \quad \text{for } i = 1, \dots, 4 \quad (7-a)$$

$$\phi_i^2 = \phi_i^2 \{ x^1, \theta^2 \} \quad \text{for } i = 1, \dots, 4 \quad (7-b)$$

$$\phi_i^3 = \phi_i^3 \{ x^2, \theta^3 \} \quad \text{"} \quad (7-c)$$

By successively substituting a pair of equations (6-2) and (7-a), then equations (6-b) and (7-b), and then equations (6-c) and (7-c) into equation (2) it is possible to eliminate all the dependent variables, and the objective function can ultimately be expressed in the following form

$$S = f(\theta_1^1, \theta_3^1, \theta_1^2, \theta_3^2) \quad (8)$$

This equation can then be differentiated to give

$$dS = \left(\frac{\partial S}{\partial \theta_1^1}\right) d\theta_1^1 + \left(\frac{\partial S}{\partial \theta_3^1}\right) d\theta_3^1 + \left(\frac{\partial S}{\partial \theta_1^2}\right) d\theta_1^2 + \left(\frac{\partial S}{\partial \theta_3^2}\right) d\theta_3^2 \quad (9)$$

On comparing equation (9) with equation (5) it is seen that $\left(\frac{\partial S}{\partial \theta_1^1}\right)$, $\left(\frac{\partial S}{\partial \theta_3^1}\right)$, $\left(\frac{\partial S}{\partial \theta_1^2}\right)$ and $\left(\frac{\partial S}{\partial \theta_3^2}\right)$, correspond respectively to [A], [B], [C], and [D] in equation (5). When all the independent variables are unbounded, the optimal policy can be obtained by setting these differentials equal to zero.

This equation will be compared with the equivalent expression derived by the second approach, which may facilitate the identification of the significance of some terms to be derived.

2. Differentiation followed by Substitution. Upon differentiating the objective function and the performance equations and the constraint equations, the following relations are obtained:

$$dS = \sum_{i=1}^7 C_i dx_i^3 \quad (10)$$

$$dx_i^3 = \sum_{j=1}^7 \frac{\partial x_i^3}{\partial x_j^2} dx_j^2 + \sum_{k=1}^6 \frac{\partial x_i^3}{\partial \theta_k^3} d\theta_k^3, \quad i = 1, \dots, 7 \quad (11-a)$$

$$dx_i^2 = \sum_{j=1}^7 \frac{\partial x_i^2}{\partial x_j^1} dx_j^1 + \sum_{k=1}^6 \frac{\partial x_i^2}{\partial \theta_k^2} d\theta_k^2, \quad " \quad (11-b)$$

$$dx_i^1 = \sum_{k=1}^6 \frac{\partial x_i^1}{\partial \theta_k^1} d\theta_k^1 \quad " \quad (11-c)$$

$$\text{and } d\phi_i^3 = \sum_{j=1}^7 \frac{\partial \phi_i^3}{\partial x_j^2} dx_j^2 + \sum_{k=1}^6 \frac{\partial \phi_i^3}{\partial \theta_k^3} d\theta_k^3 = 0, \quad i = 1, \dots, 4 \quad (12-a)$$

$$d\phi_i^2 = \sum_{j=1}^7 \frac{\partial \phi_i^2}{\partial x_j^1} dx_j^1 + \sum_{k=1}^6 \frac{\partial \phi_i^2}{\partial \theta_k^2} d\theta_k^2 = 0, \quad i = 1, \dots, 4 \quad (12-b)$$

$$d\phi_i^1 = \sum_{k=1}^6 \frac{\partial \phi_i^1}{\partial \theta_k^1} d\theta_k^1 = 0, \quad i = 1, \dots, 4 \quad (12-c)$$

Theoretically, an equation in the form of equation (5) can be obtained by successively substituting equations (11-a) and (12-a), equations (11-b) and (12-b), and equations (11-c) and (12-c) into equation (10). But such substitutions are impossible in practice for a complex system. An efficient way for handling this situation is described as follows.

For each state variable x_i^n , define an adjoint variable z_i^n and, for each constraint equation ϕ_j^n , define a Lagrange multiplier λ_j^n and then define a Hamiltonian function H^n as

$$H^n = \sum_{i=1}^7 z_i^n x_i^n + \sum_{j=1}^4 \lambda_j^n \phi_j^n \quad (13)$$

It will be assumed that z_i^n , λ_j^n , and H^n so defined are nontrivial.

For the last stage ($N = 3$), this is

$$H^3 = \sum_{i=1}^7 z_i^3 x_i^3 + \sum_{j=1}^4 \lambda_j^3 \phi_j^3 \quad (14)$$

Since ϕ_j^n 's are zero, these equations are equivalent to

$$H^n = \sum_{i=1}^7 z_i^n x_i^n \quad (13-a)$$

and

$$H^3 = \sum_{i=1}^7 z_i^3 x_i^3 \quad (14-a)$$

respectively. Equations (13) and (13-a), and (14) and (14-a) will be used interchangeably.

Differentiating equations (13) and (14) gives

$$dH^n = \sum_{i=1}^7 z_i^n dx_i^n + \sum_{j=1}^4 \lambda_j^n d\phi_j^n \quad (15)$$

and

$$dH^3 = \sum_{i=1}^7 z_i^3 dx_i^3 + \sum_{j=1}^4 \lambda_j^3 d\phi_j^3 \quad (16)$$

In these differentiations, z_i^n and λ_j^n are, by definition, kept constant. Since $d\phi_j^n = 0$, these equations are equivalent to

$$dH^n = \sum_{i=1}^7 z_i^n dx_i^n \quad (15-a)$$

and

$$dH^3 = \sum_{i=1}^7 z_i^3 dx_i^3 \quad (16-a)$$

respectively. Equations (15) and (15-a), and (16) and (16-a) will be used interchangeably.

The adjoint variables for the last stage, z_i^N 's, defined in such a way that

$$dS = dH^N \quad (17)$$

$$\text{or} \quad \sum C_i^N \cdot dx_i^N = \sum z_i^N \cdot dx_i^N \quad (17-a)$$

Therefore, the adjoint variables associated with x_i^N may be defined as

$$z_i^N = C_i^N \quad (18)$$

In the so called fixed end-point problem, however, one or more of the x_i^N 's are fixed, and for those variables we have

$$dx_i^N = 0.$$

The adjoint variables associated with these state variables can have any value and yet maintain the identity represented by equation (17). The problem of defining the z_i^N associated with a fixed state variable x_i^N will be discussed later in this section.

Substituting equations (11-a) and (12-a) into equation (16) gives

$$dS = dH^3 = \sum_{k=1}^7 \left[\sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial x_k^2} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial x_k^2} \right] dx_k^2 + \sum_{\ell=1}^4 \left[\sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta^3} \right] d\theta^3 \quad (19)$$

Before further substitutions, it is convenient to introduce Z_k^{n-1} as follows:

$$z_k^{n-1} = \sum_{i=1}^7 z_i^n \frac{\partial x_i^n}{\partial x_k^{n-1}} + \sum_{j=1}^4 \lambda_j^n \frac{\partial \phi_j^n}{\partial x_k^{n-1}} \quad (20)$$

Note that

$$\frac{\partial H^n}{\partial \theta_l^n} = \sum_{i=1}^7 z_i^n \frac{\partial x_i^n}{\partial \theta_l^n} + \sum_{j=1}^4 \lambda_j^n \frac{\partial \phi_j^n}{\partial \theta_l^n} \quad (21)$$

With these definitions, equation (19) becomes

$$dH^3 = \sum_{k=1}^7 z_k^2 dx_k^2 + \sum_{l=1}^4 \frac{\partial H^3}{\partial \theta_l^3} d\theta_l^3 \quad (22)$$

By introducing equation (15-a), the above equation can be written as

$$dH^3 = dH^2 + \sum_{l=1}^4 \frac{\partial H^3}{\partial \theta_l^3} d\theta_l^3$$

or

$$dH^3 = dH^2 + \sum_{j=1}^4 \frac{\partial H^3}{\partial \theta_j^3} d\theta_j^3 \quad (23)$$

Following similar derivations we obtain,

$$dH^2 = dH^1 + \sum_{j=1}^4 \frac{\partial H^2}{\partial \theta_j^2} d\theta_j^2 \quad (24)$$

and

$$dH^1 = dH^0 + \sum_{j=1}^4 \frac{\partial H^1}{\partial \theta_j^1} d\theta_j^1 = \sum_{j=1}^4 \frac{\partial H^1}{\partial \theta_j^1} d\theta_j^1 \quad (25)$$

$dH^0 = 0$ because all dx_i^0 's are zero.

By adding equations (23), (24), and (25), one obtains

$$dS = dH^3 = \sum_{j=1}^6 \frac{\partial H^3}{\partial \theta_j^3} d\theta_j^3 + \sum_{j=1}^6 \frac{\partial H^2}{\partial \theta_j^2} d\theta_j^2 + \sum_{j=1}^6 \frac{\partial H^1}{\partial \theta_j^1} d\theta_j^1 \quad (26)$$

The above equation contains 18 $d\theta_j^n$ terms, and most of the θ_j^n 's are dependent variables except 4 terms. Therefore, the above equation should be distinguished from equation (5), which contains only the differentials of the independent variables.

Since it is assumed that θ_3^3 is a given value, and $d\theta_3^3 = 0$, Equation (26) then contains 17 $d\theta_j^n$ terms, from which 13 terms must be eliminated in order to reduce equation (26) to equation (5).

This can be done by suitably selecting the following adjoint variable and Lagrange multipliers.

1. z_1^3 which is associated with x_1^3
2. $\lambda_1^1, \lambda_2^1, \lambda_3^1, \lambda_4^1; \lambda_1^2, \lambda_2^2, \lambda_3^2, \lambda_4^2; \lambda_1^3; \lambda_2^3, \lambda_3^3$ and λ_4^3 .

z_i^3 and λ_i^n 's are chosen so that

$$\frac{\partial H^n}{\partial \theta_i^n} = 0 \quad (27)$$

for all dependent θ_i^n 's. When z_1^3 and λ_i^n 's are so chosen to satisfy equation (27), equation (26) is reduced to

$$dS = dH^3 = \frac{\partial H^1}{\partial \theta_1^1} d\theta_1^1 + \frac{\partial H^1}{\partial \theta_3^1} d\theta_3^1 + \frac{\partial H^2}{\partial \theta_1^2} d\theta_1^2 + \frac{\partial H^2}{\partial \theta_3^2} d\theta_3^2 \quad (28)$$

On comparing equations (5), (9) and (28), the following relations are obtained:

$$[A] = \left(\frac{\partial S}{\partial \theta_1^1} \right) = \left(\frac{\partial H^1}{\partial \theta_1^1} \right) \quad (28-a)$$

$$[B] = \left(\frac{\partial S}{\partial \theta_3^1} \right) = \left(\frac{\partial H^1}{\partial \theta_3^1} \right) \quad (28-b)$$

$$[C] = \left(\frac{\partial S}{\partial \theta_1^2} \right) = \left(\frac{\partial H^2}{\partial \theta_1^2} \right) \quad (28-c)$$

$$[D] = \left(\frac{\partial S}{\partial \theta_3^2} \right) = \left(\frac{\partial H^2}{\partial \theta_3^2} \right) \quad (28-d)$$

The selection of z_1^3 and λ_i^n 's as represented by equation (27) can be written in an extended form as follows.

1. $z_1^3, \lambda_1^3, \lambda_2^3, \lambda_3^3, \lambda_4^3$ are chosen so as to satisfy the following relations.

$$\frac{\partial H^3}{\partial \theta_1^3} = \sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta_1^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta_1^3} = 0 \quad (29-a)$$

$$\frac{\partial H^3}{\partial \theta_2^3} = \sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta_2^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta_2^3} = 0 \quad (29-b)$$

$$\frac{\partial H^3}{\partial \theta_4^3} = \sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta_4^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta_4^3} = 0 \quad (29-c)$$

$$\frac{\partial H^3}{\partial \theta_5^3} = \sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta_5^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta_5^3} = 0 \quad (29-d)$$

$$\frac{\partial H^3}{\partial \theta_6^3} = \sum_{i=1}^7 z_i^3 \frac{\partial x_i^3}{\partial \theta_6^3} + \sum_{j=1}^4 \lambda_j^3 \frac{\partial \phi_j^3}{\partial \theta_6^3} = 0 \quad (29-e)$$

$\frac{\partial H^3}{\partial \theta_3^3}$ is not shown because θ_3^3 is a constant.

2. λ_1^2 , λ_2^2 , λ_3^2 and λ_4^2 are so chosen as to satisfy the following relations.

$$\frac{\partial H^2}{\partial \theta_2^2} = \sum_{i=1}^7 z_i^2 \frac{\partial x_i^2}{\partial \theta_2^2} + \sum_{j=1}^4 \lambda_j^2 \frac{\partial \phi_j^2}{\partial \theta_2^2} = 0 \quad (30-a)$$

$$\frac{\partial H^2}{\partial \theta_4^2} = \sum_{i=1}^7 z_i^2 \frac{\partial x_i^2}{\partial \theta_4^2} + \sum_{j=1}^4 \lambda_j^2 \frac{\partial \phi_j^2}{\partial \theta_4^2} = 0 \quad (30-b)$$

$$\frac{\partial H^2}{\partial \theta_5^2} = \sum_{i=1}^7 z_i^2 \frac{\partial x_i^2}{\partial \theta_5^2} + \sum_{j=1}^4 \lambda_j^2 \frac{\partial \phi_j^2}{\partial \theta_5^2} = 0 \quad (30-c)$$

$$\frac{\partial H^2}{\partial \theta_6^2} = \sum_{i=1}^7 z_i^2 \frac{\partial x_i^2}{\partial \theta_6^2} + \sum_{j=1}^4 \lambda_j^2 \frac{\partial \phi_j^2}{\partial \theta_6^2} = 0 \quad (30-d)$$

3. λ_1^1 , λ_2^1 , λ_3^1 and λ_4^1 are so chosen as to satisfy the following relations.

$$\frac{\partial H^1}{\partial \theta_2^1} = \sum_{i=1}^7 z_i^1 \frac{\partial x_i^1}{\partial \theta_2^1} + \sum_{j=1}^4 \lambda_j^1 \frac{\partial \phi_j^1}{\partial \theta_2^1} = 0 \quad (31-a)$$

$$\frac{\partial H^1}{\partial \theta_4^1} = \sum_{i=1}^7 z_i^1 \frac{\partial x_i^1}{\partial \theta_4^1} + \sum_{j=1}^4 \lambda_j^1 \frac{\partial \phi_j^1}{\partial \theta_4^1} = 0 \quad (31-b)$$

$$\frac{\partial H^1}{\partial \theta_5^1} = \sum_{i=1}^7 z_i^1 \frac{\partial x_i^1}{\partial \theta_5^1} + \sum_{j=1}^4 \lambda_j^1 \frac{\partial \phi_j^1}{\partial \theta_5^1} \quad (31-c)$$

$$\frac{\partial H^1}{\partial \theta_6^1} = \sum_{i=1}^7 z_i^1 \frac{\partial x_i^1}{\partial \theta_6^1} + \sum_{j=1}^4 \lambda_j^1 \frac{\partial \phi_j^1}{\partial \theta_6^1} \quad (31-d)$$

With z_1^3 and λ_i^n 's evaluated to satisfy equations (29), (30) and (31), dS is represented by equation (28).

When z_1^3 and λ_i^n 's are evaluated as described, and if the independent variables are unbounded, the locally optimal set of $\{\theta_1^1, \theta_3^1, \theta_1^2, \theta_3^2\}$, if it exists, is the set which satisfies the following stationary conditions:

$$\frac{\partial H^1}{\partial \theta_1^1} = \frac{\partial H^1}{\partial \theta_3^1} = \frac{\partial H^2}{\partial \theta_1^2} = \frac{\partial H^2}{\partial \theta_3^2} = 0 \quad (32)$$

where $\frac{\partial H^n}{\partial \theta_6^n}$ is defined by equation (21).

III. OPTIMIZATION OF A THREE-STAGES GAS COMPRESSION SYSTEM

The discussion in the preceding section applies to a multi-stage (3-stage) gas compression system, and relations to be used in the optimization study are developed.

1. Third stage

All the decision variables $\theta_1^3, \theta_2^3, \theta_3^3, \theta_4^3, \theta_5^3, \theta_6^3$, at the third stage are actually dependent variables, because there are four equality constraints and both x_1^3 and θ_3^3 are given. The objective function is defined as

$$S = x_7^3 \quad (33)$$

and the Hamiltonian function is defined as

$$H^3 = \sum_{i=1}^7 z_i^3 x_i^3 + \sum_{j=1}^4 \lambda_j^3 \phi_j^3 \quad (34)$$

Note that, as indicated by equation (18), one has

$$z_2^3 = z_3^3 = z_4^3 = z_5^3 z_6^3 = 0 \quad (35)$$

$$z_7^3 = 1 \quad (36)$$

z_1^3 is left undecided because x_1^3 is a fixed value. z_1^3 will be evaluated along with λ_j^3 shortly.

The Hamiltonian function H^3 then becomes

$$H^3 = z_1^3 x_1^3 + x_7^3 + \lambda_1^3 \phi_1^3 + \lambda_2^3 \phi_2^3 + \lambda_3^3 \phi_3^3 + \lambda_4^3 \phi_4^3 \quad (37)$$

$z_1^3, \lambda_1^3, \lambda_2^3, \lambda_3^3, \lambda_4^3$ are to be found from the following relations [see equation (27)].

$$\frac{\partial H^3}{\partial \theta_1^3} = \frac{\partial H^3}{\partial \theta_2^3} = \frac{\partial H^3}{\partial \theta_4^3} = \frac{\partial H^3}{\partial \theta_5^3} = \frac{\partial H^3}{\partial \theta_6^3} = 0. \quad (38)$$

Equation (38) can be written in an expanded form as

$$\begin{aligned} \frac{\partial H^3}{\partial \theta_1^3} &= z_1^3 \frac{\partial x_1^3}{\partial \theta_1^3} + \frac{\partial x_1^3}{\partial \theta_1^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_1^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_1^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_1^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_1^3} = 0 \\ \frac{\partial H^3}{\partial \theta_2^3} &= z_1^3 \frac{\partial x_1^3}{\partial \theta_2^3} + \frac{\partial x_7^3}{\partial \theta_2^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_2^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_2^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_2^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_2^3} = 0 \\ \frac{\partial H^3}{\partial \theta_4^3} &= z_1^3 \frac{\partial x_1^3}{\partial \theta_4^3} + \frac{\partial x_7^3}{\partial \theta_4^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_4^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_4^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_4^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_4^3} = 0 \quad (39) \\ \frac{\partial H^3}{\partial \theta_5^3} &= z_1^3 \frac{\partial x_1^3}{\partial \theta_5^3} + \frac{\partial x_7^3}{\partial \theta_5^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_5^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_5^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_5^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_5^3} = 0 \\ \frac{\partial H^3}{\partial \theta_6^3} &= z_1^3 \frac{\partial x_1^3}{\partial \theta_6^3} + \frac{\partial x_7^3}{\partial \theta_6^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_6^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_6^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_6^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_6^3} = 0 \end{aligned}$$

Table 3 shows the functional relations of x_i^n and ϕ_i^n respectively to x_i^{n-1} and θ_i^n . As shown, many terms in the above equations can be eliminated, because there are no functional relations between the variables involved.

The above equations can be rearranged as

$$z_1^3 \frac{\partial x_1^3}{\partial \theta_1^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_1^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_1^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_1^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_1^3} = 0 \quad (40-a)$$

$$\frac{\partial x_7^3}{\partial \theta_2^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_2^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_2^3} = 0 \quad (40-b)$$

$$z_1^3 \frac{\partial x_1^3}{\partial \theta_4^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_4^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_4^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_4^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_4^3} = 0 \quad (40-c)$$

$$\frac{\partial x_7^3}{\partial \theta_5^3} + \lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_5^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_5^3} = 0 \quad (40-d)$$

$$\frac{\partial x_7^3}{\partial \theta_6^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_6^3} = 0 \quad (40-e)$$

By solving these equations simultaneous, one obtains $z_1^3, \lambda_1^3, \lambda_2^3,$

λ_3^3, λ_4^3 as follows:

$$z_1^3 = - \left(\lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_1^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_1^3} + \lambda_3^3 \frac{\partial \phi_3^3}{\partial \theta_1^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_1^3} \right) / \left(\frac{\partial x_1^3}{\partial \theta_1^3} \right) \quad (41)$$

$$\lambda_1^3 = - \left(\frac{\partial x_7^3}{\partial \theta_2^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_2^3} \right) / \left(\frac{\partial \phi_1^3}{\partial \theta_2^3} \right) \quad (42)$$

$$\begin{aligned} & \left[\frac{\partial x_7^3}{\partial \theta_5^3} \frac{\partial \phi_4^3}{\partial \theta_2^3} - \frac{\partial x_7^3}{\partial \theta_2^3} \frac{\partial \phi_4^3}{\partial \theta_5^3} \right] \\ &= \frac{\left[\frac{\partial x_7^3}{\partial \theta_5^3} \frac{\partial \phi_4^3}{\partial \theta_2^3} - \frac{\partial x_7^3}{\partial \theta_2^3} \frac{\partial \phi_4^3}{\partial \theta_5^3} \right]}{\left[\frac{\partial \phi_1^3}{\partial \theta_2^3} \frac{\partial \phi_4^3}{\partial \theta_5^3} - \frac{\partial \phi_1^3}{\partial \theta_5^3} \frac{\partial \phi_4^3}{\partial \theta_2^3} \right]} \end{aligned} \quad (43)$$

$$\lambda_2^3 = - \left(\frac{\partial x_7^3}{\partial \theta_6^3} \right) / \left(\frac{\partial \phi_2^3}{\partial \theta_6^3} \right) \quad (44)$$

$$\lambda_3^3 = \frac{\left(\lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_4^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_4^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_4^3} \right) \left(\frac{\partial x_1^3}{\partial \theta_1^3} \right) - \left(\lambda_1^3 \frac{\partial \phi_1^3}{\partial \theta_1^3} + \lambda_2^3 \frac{\partial \phi_2^3}{\partial \theta_1^3} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial \theta_1^3} \right) \left(\frac{\partial x_1^3}{\partial \theta_4^3} \right)}{\left(\frac{\partial \phi_3^3}{\partial \theta_1^3} \right) \left(\frac{\partial x_1^3}{\partial \theta_4^3} \right) - \left(\frac{\partial \phi_3^3}{\partial \theta_4^3} \right) \left(\frac{\partial x_1^3}{\partial \theta_1^3} \right)} \quad (45)$$

$$\lambda_4^3 = - \frac{\left[\frac{\partial x_7^3}{\partial \theta_2^3} \frac{\partial \phi_1^3}{\partial \theta_5^3} - \frac{\partial x_7^3}{\partial \theta_5^3} \frac{\partial \phi_1^3}{\partial \theta_2^3} \right]}{\left[\frac{\partial \phi_4^3}{\partial \theta_2^3} \frac{\partial \phi_1^3}{\partial \theta_5^3} - \frac{\partial \phi_4^3}{\partial \theta_5^3} \frac{\partial \phi_1^3}{\partial \theta_2^3} \right]} = \frac{\left[\frac{\partial x_7^3}{\partial \theta_5^3} \frac{\partial \phi_1^3}{\partial \theta_2^3} - \frac{\partial x_7^3}{\partial \theta_2^3} \frac{\partial \phi_1^3}{\partial \theta_5^3} \right]}{\left[\frac{\partial \phi_4^3}{\partial \theta_2^3} \frac{\partial \phi_1^3}{\partial \theta_5^3} - \frac{\partial \phi_4^3}{\partial \theta_5^3} \frac{\partial \phi_1^3}{\partial \theta_2^3} \right]} \quad (46)$$

2. Second Stage

Of all the decision variables, only two are truly independent and thus θ_1^2 and θ_3^2 are chosen to be the independent variables. The adjoint variables associated with the second stage are obtained from equation (20) as

$$z_1^2 = 0$$

$$z_2^2 = 0$$

$$z_3^2 = 0$$

$$\begin{aligned} z_4^2 &= z_7^3 \frac{\partial x_7^3}{\partial x_4^2} + \lambda_4^3 \frac{\partial \phi_4^3}{\partial x_4^2} = -1 [- (c_e + \psi_1 c_{HP})] + \lambda_4^3 (0.2) \\ &= (c_e + \psi_1 c_{HP}) + 0.2 \lambda_4^3 \quad (47) \end{aligned}$$

$$z_5^2 = 0$$

$$z_6^2 = -\lambda_3^3$$

$$z_7^2 = z_7^3 \frac{\partial x_7^n}{\partial x_7^{n-1}} = 1 \cdot 1 = 1$$

λ_1^2 , λ_2^2 , λ_3^2 , and λ_4^2 should be found from the following relations
[see equation (27)]

$$\frac{\partial H^2}{\partial \theta_2^2} = \frac{\partial H^2}{\partial \theta_4^2} = \frac{\partial H^2}{\partial \theta_5^2} = \frac{\partial H^2}{\partial \theta_6^2} = 0 \quad (48)$$

By writing the above equations in expanded form, simplifying by introducing functional relations from Table 3, and solving the four simultaneous equations so obtained, one arrives at

$$\lambda_2^2 = \frac{- \left\{ z_4^2 \frac{\partial x_4^2}{\partial \theta_6^2} + z_6^2 \frac{\partial x_6^2}{\partial \theta_6^2} + \frac{\partial x_7^2}{\partial \theta_6^2} \right\}}{\frac{\partial \phi_2^2}{\partial \theta_6^2}} \quad (49)$$

$$\lambda_4^2 = \frac{\left[\left(\frac{\partial x_7^2}{\partial \theta_5^2} \right) \left(\frac{\partial \phi_1^2}{\partial \theta_2^2} \right) - \left(\frac{\partial x_7^2}{\partial \theta_2^2} \right) \left(\frac{\partial \phi_1^2}{\partial \theta_5^2} \right) \right]}{\left[\left(\frac{\partial \phi_4^2}{\partial \theta_2^2} \right) \left(\frac{\partial \phi_1^2}{\partial \theta_5^2} \right) - \left(\frac{\partial \phi_4^2}{\partial \theta_5^2} \right) \left(\frac{\partial \phi_1^2}{\partial \theta_2^2} \right) \right]} \quad (50)$$

$$\lambda_1^2 = - \left(\lambda_4^2 \frac{\partial \phi_4^2}{\partial \theta_5^2} + \frac{\partial x_7^2}{\partial \theta_5^2} \right) / \left(\frac{\partial \phi_1^2}{\partial \theta_5^2} \right) \quad (51)$$

$$\lambda_3^2 = \frac{- \left(\lambda_1^2 \frac{\partial \phi_1^2}{\partial \theta_4^2} + \lambda_2^2 \frac{\partial \phi_2^2}{\partial \theta_4^2} + \lambda_4^2 \frac{\partial \phi_4^2}{\partial \theta_4^2} \right)}{\left(\frac{\partial \phi_3^2}{\partial \theta_4^2} \right)} \quad (52)$$

3. First stage

Following a derivation similar to that for the second stage, one obtains

$$z_1^1 = 0$$

$$z_2^1 = 0$$

$$z_3^1 = 0$$

$$z_4^1 = z_7^2 \frac{\partial x_7^2}{\partial x_4^1} + \lambda_4^2 \frac{\partial \phi_4^2}{\partial x_4^1} = [c_e + \psi_1 c_{HP}] + 0.2 \lambda_4^2 \quad (53)$$

$$z_5^1 = 0$$

$$z_6^1 = -\lambda_3^2$$

$$z_1^1 = z_7^2 \frac{\partial x_7^2}{\partial x_7^1} = 1 \cdot 1 = 1$$

and λ_1^1 , λ_2^1 , λ_3^1 and λ_4^1 are obtained as

$$\lambda_2^1 = \frac{- \left\{ z_4^1 \frac{\partial x_4^1}{\partial \theta_6^1} + z_6^1 \frac{\partial x_6^1}{\partial \theta_6^1} + \frac{\partial x_7^1}{\partial \theta_6^1} \right\}}{\frac{\partial \phi_2^1}{\partial \theta_6^1}} \quad (54)$$

$$\lambda_4^1 = \frac{\left(\frac{\partial x_7^1}{\partial \theta_5^1} \right) \left(\frac{\partial \phi_1^1}{\partial \theta_2^1} \right) - \left(\frac{\partial x_7^1}{\partial \theta_2^1} \right) \left(\frac{\partial \phi_1^1}{\partial \theta_5^1} \right)}{\left(\frac{\partial \phi_4^1}{\partial \theta_2^1} \right) \left(\frac{\partial \phi_1^1}{\partial \theta_5^1} \right) - \left(\frac{\partial \phi_4^1}{\partial \theta_5^1} \right) \left(\frac{\partial \phi_1^1}{\partial \theta_2^1} \right)} \quad (55)$$

$$\lambda_1^1 = - \left(\lambda_4^1 \frac{\partial \phi_4^1}{\partial \theta_5^1} \frac{\partial x_7^1}{\partial \theta_5^1} \right) / \left(\frac{\partial \phi_1^1}{\partial \theta_5^1} \right) \quad (56)$$

$$\lambda_3^1 = \frac{- \left(\lambda_1^1 \frac{\partial \phi_1^1}{\partial \theta_4^1} + \lambda_2^1 \frac{\partial \phi_2^1}{\partial \theta_4^1} + \lambda_4^1 \frac{\partial \phi_4^1}{\partial \theta_4^1} \right)}{\left(\frac{\partial \phi_3^1}{\partial \theta_4^1} \right)} \quad (57)$$

With the z 's and λ 's determined as above, the independent decision derivatives of the Hamiltonian functions, $\frac{\partial H^2}{\partial \theta_1^2}$, $\frac{\partial H^2}{\partial \theta_3^2}$, $\frac{\partial H^1}{\partial \theta_1^1}$, $\frac{\partial H^1}{\partial \theta_3^1}$ can be obtained as

$$\frac{\partial H^2}{\partial \theta_1^2} = \lambda_1^2 \frac{\partial \phi_1^2}{\partial \theta_1^2} + \lambda_2^2 \frac{\partial \phi_2^2}{\partial \theta_1^2} + \lambda_3^2 \frac{\partial \phi_3^2}{\partial \theta_1^2} + \lambda_4^2 \frac{\partial \phi_4^2}{\partial \theta_1^2} \quad (58)$$

$$\frac{\partial H^2}{\partial \theta_3^2} = z_4^2 \frac{\partial x_4^2}{\partial \theta_3^2} + z_6^2 \frac{\partial x_6^2}{\partial \theta_3^2} + \frac{\partial x_7^2}{\partial \theta_3^2} + \lambda_2^2 \frac{\partial \phi_2^2}{\partial \theta_3^2} \quad (59)$$

$$\frac{\partial H^1}{\partial \theta_1^1} = \lambda_1^1 \frac{\partial \phi_1^1}{\partial \theta_1^1} + \lambda_2^1 \frac{\partial \phi_2^1}{\partial \theta_1^1} + \lambda_3^1 \frac{\partial \phi_3^1}{\partial \theta_1^1} + \lambda_4^1 \frac{\partial \phi_4^1}{\partial \theta_1^1} \quad (60)$$

$$\frac{\partial H^1}{\partial \theta_3^1} = z_4^1 \frac{\partial x_4^1}{\partial \theta_3^1} + z_5^1 \frac{\partial x_6^1}{\partial \theta_3^1} + \frac{\partial x_7^1}{\partial \theta_3^1} + \lambda_2^1 \frac{\partial \phi_2^1}{\partial \theta_3^1} \quad (61)$$

When the independent decision variables θ_1^1 , θ_3^1 , θ_1^2 , θ_3^2 are at the local optimum values, these derivations, if they exist, should be zero.

The above derivations show how z_1^1 , z_2^1 , z_3^1 , z_4^1 , z_5^1 , z_6^1 , z_7^1 ; z_1^2 , z_2^2 , z_3^2 , z_4^2 , z_5^2 , z_6^2 , z_7^2 ; z_2^3 , z_3^3 , z_4^3 , z_5^3 , z_6^3 , z_7^3 can be evaluated and how z_1^3 ; λ_1^3 , λ_2^3 , λ_3^3 , λ_4^3 ; λ_1^2 , λ_2^2 , λ_3^2 , λ_4^2 ; λ_1^1 , λ_2^1 , λ_3^1 , λ_4^1 ;

$\frac{\partial H^1}{\partial \theta_1^1}$, $\frac{\partial H^1}{\partial \theta_3^1}$, $\frac{\partial H^2}{\partial \theta_1^2}$ and $\frac{\partial H^2}{\partial \theta_3^2}$ are related to the decision derivatives of the state variables and constraint functions, $\frac{\partial x_i^n}{\partial \theta_l^n}$ and $\frac{\partial \phi_i^n}{\partial \theta_l^n}$.

The decision derivatives of x_i^n and ϕ_j^n are functions of decision variables only (both independent and dependent) and are summarized in Part B of Chapter 4.

With these relations available, the optimization study for determining locally optimal conditions of a multistage gas compression system can be stated as follows:

The optimization study of a multistage gas compression system is to find the set of values for θ_1^1 , θ_3^1 , θ_1^2 and θ_3^2 which makes $\frac{\partial H^1}{\partial \theta_1^1}$, $\frac{\partial H^1}{\partial \theta_3^1}$, $\frac{\partial H^2}{\partial \theta_1^2}$ and $\frac{\partial H^2}{\partial \theta_3^2}$ as calculated by equations (58), (59), (60), and (61) zero, when z_i^n 's and λ_j^n 's are evaluated by the relations derived in this section. It is theoretically possible to find the optimum set by simultaneously solving the performance equations and all the relations derived in this section. Such simultaneous solution is practically impossible. Therefore, an iterative numerical solution will be employed.

IV. ITERATIVE NUMERICAL SOLUTION FOR THE OPTIMIZATION OF A MULTISTAGE GAS COMPRESSION SYSTEM

The iterative numerical solution used in the present study consists of the following steps:

- Step 1. Assume a set of numerical values for the independent decision variables θ_1^1 , θ_3^1 , θ_1^2 , and θ_3^2 .
- Step 2. Find the numerical values for all the remaining decision variables and the state variables by the relations described in Part A of Chapter 4.

- Step 3. Calculate the numerical values for $\frac{\partial x_i^n}{\partial \theta_l^n}$ and $\frac{\partial \phi_i^n}{\partial \theta_l^n}$ by substituting the numerical values of the decision variables and state variables into the relations derived in Part B of Chapter 4.
- Step 4. Calculate the numerical values for z_i^n and λ_i^n by the relations derived in this section.
- Step 5. Calculate the numerical values $\frac{\partial H^1}{\partial \theta_1^1}$, $\frac{\partial H^1}{\partial \theta_3^1}$, $\frac{\partial H^2}{\partial \theta_1^2}$ and $\frac{\partial H^2}{\partial \theta_3^2}$ by equations (58), (59), (60) and (61).
- Step 6. Check if the assumed set of (θ_i^n) is the optimal policy by noting that all values of $\frac{\partial H^n}{\partial \theta_i^n}$ for all the independent decision variables are zero or less than the allowable errors preassigned to them.
- Step 7. When the optimal condition is not reached a revised set of decision variables should be assumed and the above computations should be repeated. The new set of decision variables may be automatically assumed by giving a set of $(\Delta \theta_i^n)$ and input data to the computer. This set of $(\Delta \theta_i^n)$ may be varied at different stages of computation. For example, we may use larger values for $\Delta \theta_i^n$ at the beginning and use smaller values as the iteration converges.

The new decision variable is obtained by

$$\left(\theta_i^n \right)_{\text{revised}} = \left(\theta_i^n \right)_{\text{old}} + \left(\Delta \theta_i^n \right) \quad (62)$$

For a particular θ_i^n , the sign before $\Delta\theta_i^n$ is defined as follows:

$$\text{when } \frac{\partial H^n}{\partial \theta_i^n} > 0 \quad \text{use (-) sign,} \quad (63)$$

$$\text{when } \frac{\partial H^n}{\partial \theta_i^n} < 0 \quad \text{use (+) sign.} \quad (64)$$

assuming that in the region of computations, the sign of $\frac{\partial S}{\partial \theta_i}$ and $\frac{\partial H}{\partial \theta_i}$ are always identical as suggested by equations (28-a), (28-b), (28-c), and (28-d). Note that this assumption is not necessarily valid in every point of the region especially at the very close vicinity of a stationary point. The reasons for this rule can be explained by referring to a one-dimensional minimum seeking problem. Referring to Fig. 9, it is readily seen that the slope of the S-curve, $(\frac{\partial S}{\partial \theta})$ is a positive value when θ exceeds the optimum value, $\bar{\theta}$. In other words, when $\frac{\partial S}{\partial \theta}$ is positive the sign before $\Delta\theta$ in equation (62) should be negative in order to approach the optimum value. Conversely, when $\frac{\partial S}{\partial \theta}$ is negative, the θ used is still lower than $\bar{\theta}$. Therefore, the sign should be positive. Incidentally, in a maximum seeking problem the rule should be reversed as follows:

$$\text{when } \frac{\partial H^n}{\partial \theta_i^n} > 0 \quad \text{use (+) sign,}$$

$$\text{when } \frac{\partial H^n}{\partial \theta_i^n} < 0 \quad \text{use (-) sign.}$$

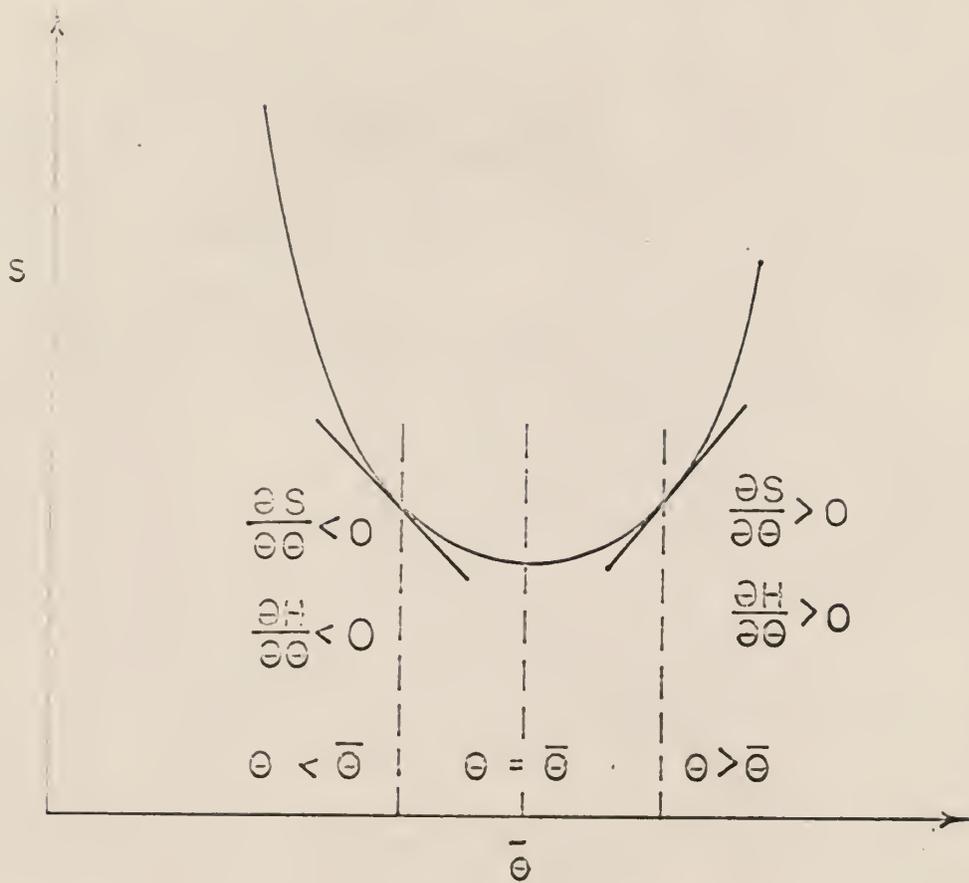


Fig. 9. One dimensional optimum search.

It has to be kept in mind, when the second order variational effect becomes appreciable in comparison to the first order variational effect, the signs of $\frac{\partial H^n}{\partial \theta_i^n}$ and $\frac{\partial S}{\partial \theta_i^n}$ may be reversed and consequently the rule of selecting the sign of $\frac{\partial H^n}{\partial \theta_i^n}$ may have to be reversed.

Step 8. When the above computation is repeated, a point will be reached where all the $\frac{\partial H}{\partial \theta}$ change their signs between the m-th and (m + 1)-th iteration. The optimum policy then lies between the two sets of decision variables used in the m-th and (m+1)th iterations.

In order to find the optimum more precisely, another set of $(\Delta\theta)$ with smaller values assigned to $\Delta\theta_i^n$ may be used and the above computation repeated to again locate the point where a complete reversal in sign of $\frac{\partial H}{\partial \theta}$ takes place. By successively assigning smaller values for the $(\Delta\theta)$ set, we can approach the accuracy that is desired.

Step 2 in the above list requires further explanation. In a multistage gas compression problem, inlet conditions and outlet conditions are given. Therefore θ_3^0 , x_1^0 , θ_3^3 and x_1^3 are given values, and x_7^0 is assumed to be zero in this study. Due to step 1, θ_1^1 , θ_3^1 , θ_1^2 and θ_3^2 are given values for each iteration. In step 2, numerical values are to be found for all the remaining decision variables and all the state variables. The computation consists of the following steps.

1. Computation of θ_6^0 , x_4^0 and x_6^0 in stage 0 (hypothetical stage)
 - 1-a. Knowing θ_3^0 , x_1^0 , calculate θ_6^0 by equation (IV-3).
 - 1-b. Knowing θ_3^0 and θ_6^0 , calculate x_4^0 by equation (IV-6).
 - 1-c. Knowing θ_3^0 and θ_6^0 , calculate x_6^0 by equation (IV-8).

2. Computation of θ_i^1 and x_j^1 in the first stage.
 - 2-a. x_5^1 is equated to x_6^0
 - 2-b. Knowing x_5^1 and θ_1^1 , calculate θ_4^1 by equation (IV-7).
 - 2-c. Knowing θ_1^1 and θ_4^1 , calculate x_1^1 by equation (IV-1).
 - 2-d. Knowing θ_1^1 and θ_4^1 , calculate x_2^1 by equation (IV-4).
 - 2-e. Knowing x_4^0 and x_2^1 , calculate x_3^1 by equation (IV-16).
 - 2-f. Knowing x_1^1 and x_3^1 calculate θ_2^1 and θ_5^1 by equations (IV-2) and (IV-5).
 - 2-g. Knowing θ_3^1 and x_1^1 calculate θ_6^1 by equation (IV-3).
 - 2-h. Knowing θ_3^1 and θ_6^1 calculate x_4^1 by equation (IV-6).
 - 2-i. Knowing θ_3^1 and θ_6^1 calculate x_6^1 by equation (IV-8).
 - 2-j. Knowing all the θ 's and x 's calculate x_7^1 by equation (IV-9).

3. Computation of θ_i^2 and x_j^2 in the second stage. The computation is similar to the computation for the first stage.

4. Computation of θ_i^3 and x_j^3 in the third stage.
 - 4-a. Equate x_5^3 to x_6^2
 - 4-b. Knowing θ_3^3 and x_1^3 (both are given values in an optimization problem), find θ_6^3 by equation (IV-3).
 - 4-c. Knowing θ_3^3 and θ_6^3 , calculate x_4^3 by equation (IV-6)

- 4-d. Knowing θ_3^3 and θ_6^3 , calculate x_6^3 by equation (IV-8).
- 4-e. Knowing x_1^3 and x_5^3 calculate θ_1^3 and θ_4^3 by equations (IV-1) and (IV-7).
- 4-f. Knowing θ_1^3 and θ_4^3 , calculate x_2^3 by equation (IV-4).
- 4-g. Knowing x_2^3 and x_4^3 calculate x_3^3 by equation (IV-16).
- 4-h. Knowing x_1^3 and x_3^3 calculate θ_2^3 and θ_5^3 by equations (IV-2) and IV-5).
- 4-i. Knowing x_i^3 's and θ_j^3 's, calculate x_7^3 by equation (IV-9).

In the above computations, the computations belonging to the following two types require trial calculations.

1. Type 1. Knowing θ_k^n , x_i^n calculate for θ_j^n .

Examples are computations 1-a, 2-b, 2-g, and 4-b in the above list. Transformation equations are written in the form of

$$x_i^n = T_i^n(\theta_k^n, \theta_j^n),$$

and the function is implicit with respect to θ_k^n and θ_j^n .

Therefore, in the numerical computation by a digital computer, the following steps have been taken

- a. Assume a value for θ_j^n .
- b. Compute an x_i^n value from the above equation, and record the result as (x_i^n) calculated
- c. Calculate Δx_i^n value which is defined as

$$\Delta x_i^n = (x_i^n)_{\text{known}} - (x_i^n)_{\text{calculated}}$$

- d. If Δx is within the preassigned allowable error record the assumed θ_j^n as the root required.

- e. If Δx is greater than the preassigned allowable error, assume a new value of θ_j^n by

$$(\theta_j^n)_{\text{new}} = (\theta_j^n)_{\text{old}} \pm \Delta \theta_j^n \quad (65)$$

The sign ahead of $\Delta \theta_j^n$ should be decided by the nature of transformation equation. The $(\theta_j^n)_{\text{new}}$ value is considered as the new assumed value and all the steps repeated.

One may start with a large value of $\Delta \theta_j^n$ at the beginning and use a successively smaller value for the $\Delta \theta_j^n$ as the computation converges. One way is to compare Δx_i^n values in two successive computations. When the Δx_i^n value changes its sign during two successive computations, halve the $\Delta \theta_j^n$ value. This approach is incorporated in the optimization calculations of CO₂ compression problems.

Note that other one dimension root finding methods such as Newton's method and Fibnachi's method, which are more efficient than the interval halving method mentioned above, can also be used.

2. Type 2. Knowing x_i^n and x_j^n calculate θ_k^n and θ_l^n . Examples are computations of equation (2-f), (3-f), (4-e), and (4-h) in the above list.

Transformation equations are written in the form of

$$x_i^n = T_i^n(\theta_k^n, \theta_l^n) \quad (A)$$

$$x_j^n = T_j^n(\theta_k^n, \theta_l^n) \quad (B)$$

The following computational steps have been taken:

- a. Assume a value for θ_k^n
- b. Knowing θ_k^n and x_i^n , calculate θ_l^n by equation (A) and by the steps described in connection with the Type 1 problem.
- c. Using values of θ_k^n (from step a) and θ_l^n (from step b) compute an x_j^n value by equation (B), and record the result as $(x_j^n)_{\text{calculated}}$
- d. Calculate the Δx_j^n value which is defined as

$$\Delta x_j^n = (x_j^n)_{\text{known}} - (x_j^n)_{\text{calculated}}$$

- e. Similar to step (d) for Type 1.
- f. Similar to step (e) for Type 1.

The relations derived and the methods described in this chapter are used in solving various problems set up for compressing CO₂ gas by a three-stage compression. The results of the computations are described in the next chapter.

CHAPTER 6. OPTIMIZATION STUDY OF A MULTISTAGE (3-stage)
GAS COMPRESSION PROCESS OF CARBON DIOXIDE TO
VARIOUS DISCHARGE CONDITIONS

1. INTRODUCTION

The procedure developed in Chapter 5 is perfectly general and can be applied to the optimization study of compressing any gas from any inlet conditions to any discharge conditions, provided equations of state are available. The equations of state developed by Hirshfelder et al. are quite general and accurate. According to their approach, the field is divided into three regions; viz. low density gas (Region I), high density gas (Region II) and liquid (Region III). Gas compression in industrial processes may span two regions or even three regions. The procedures developed can handle even the most complex problem which can be formulated.

In order to illustrate the procedures and to demonstrate the actual saving realizable by the application of the optimization technique developed in this study as compared with the conventional approach, the optimization technique has been applied to a multi-stage CO₂ gas compression problem in which the gas remains in Region I only.

In order to assist visualization of the procedure and showing how the successive iterations converge to the optimum condition, a two dimensional problem is formulated by fixing θ_3^1 and θ_3^2 and considering θ_1^1 and θ_1^2 as the two independent variables controlling the process. Optimization study of a two-dimensional problem is described in Section II.

Several optimization problems have been set up by varying the discharge conditions. These problems have been solved and the results of the calculations are described in Section III.

II. NUMERICAL SOLUTION OF A TWO DIMENSIONAL PROBLEM

The two dimensional problem is stated as follows:

CO₂ gas is compressed by a 3-stage gas compression system from 85 °F and 14.7 Psi to the discharge condition of 140 °F and 1700 Psi. The gas is cooled to 100 °F after the first and second stage compressions. The constants used in the problem are summarized in Table 4. Find the optimum discharge pressures from the first and second stage compressions and the cost under the optimum operating condition.

The two parameter suboptimization problem can be solved by the discrete analog of the maximum principle according to the numerical computation procedure summarized in Chapter 5. Starting from a trial set of independent variables $\{T_1^1, T_2^1\}$ or equivalently $\{\theta_1^1, \theta_1^2\}$, the values of $\frac{\partial H^1}{\partial \theta_1^1}$ and $\frac{\partial H^2}{\partial \theta_1^2}$ can be calculated and use these values and the sign of the derivatives as a guide in selecting a new trial set of decision variables. The successive iteration ultimately converges to the optimum condition for the problem under consideration.

With a two dimensional problem, the contour lines of constant gas compression cost can be shown graphically and show how the locus of successive iterations shown converges to the same optimal condition for different starting trial sets of T_1^1, T_2^1 or equivalently $\{\theta_1^1, \theta_1^2\}$. It should be noted that the present technique

Table 4. Numerical Values for the Constants

b	$= 0.1983$	P_o	$= 14.7 \text{ lb/in}^2$
b'	$= 0.739$	P_c	$= 1066 \text{ lb/in}^2$
C_e	$= 2.94 \times 10^{-6} \text{ \$/Btu}$	R	$= 1.987 \text{ Btu/lb-mole R}$
C_H	$= 7 \text{ \$/ft}^2$	S^o	$= 62.26 \text{ Btu/lb-mole R}$
C_{HP}	$= 100 \text{ \$/hp.hr}$		at 492^oR
	$= 3.93 \times 10^{-2} \text{ \$/Btu}$		14.7 psi (Ref 14)
$(C_p)_w$	$= 1$	T_o	$= 492 \text{ R}$
C_w	$= 1.5 \times 10^{-6} \text{ \$/lb}$	T_c	$= 547.8 \text{ R}$
H^o	$= 1340 \text{ Btu/lb-mole}$		
	at $492^o\text{R}, 14.7 \text{ psi}$	$(t_w)_o$	$= \left(\frac{120 + 460}{T_c} \right) = 1.050$
	(Ref 14)	$(t_w)_i$	$= \left(\frac{85 + 460}{T_c} \right) = 0.995$
k_o	$= 5.5$	U	$= 5 \text{ Btu/ft.}^2\text{hr.}^o\text{F}$
k_1	$= 1.43$	V_c	$= 0.0342 \text{ cu. ft/lb.}$
k_2	$= 1.33$	Z_c	$= 0.275$
k_3	$= 1.478$	ψ_1, ψ_2	$= 9.4 \times 10^{-6}$
k_4	$= 0.794$		

Note: Source of cost data (Ref. 24)

is distinct from the gradient technique. In the gradient technique the direction of the successive iterations are taken normal to the contour lines. In the present method, the direction of successive iterations is not necessarily normal to the contour lines.

Figure 10 shows the gas compression cost vs. T_1' at various values of T_2' . The optimum condition is found to be $T_1' = 329^\circ\text{F}$, $T_2' = 330^\circ\text{F}$, and the gas compression cost is 2.510¢/lb-mole.

Figure 11 shows the contour lines of constant CO_2 compression cost. It also shows starting from conditions represented by points 1, 1', 1'', 1''', how the successive iterations lead to the optimum condition of lowest cost.

III. RESULTS OF NUMERICAL COMPUTATION OF 3-STAGES CO_2 GAS COMPRESSION PROBLEMS

Several problems have been formulated by varying the discharge condition.

The problems are stated as follows:

CO_2 gas is compressed by a 3-stage gas compression system from 85°F and 14.7 psi to the following discharge conditions:

<u>Discharge Pressure (psi)</u>	<u>Discharge temperature ($^\circ\text{F}$)</u>
500	100, 140, 180, 220, 260
800	100, 140, 180, 220, 260
1100	100, 140, 180, 220, 260, 300
1400	140, 180, 220, 260, 300
1700	140, 180, 220, 260, 300

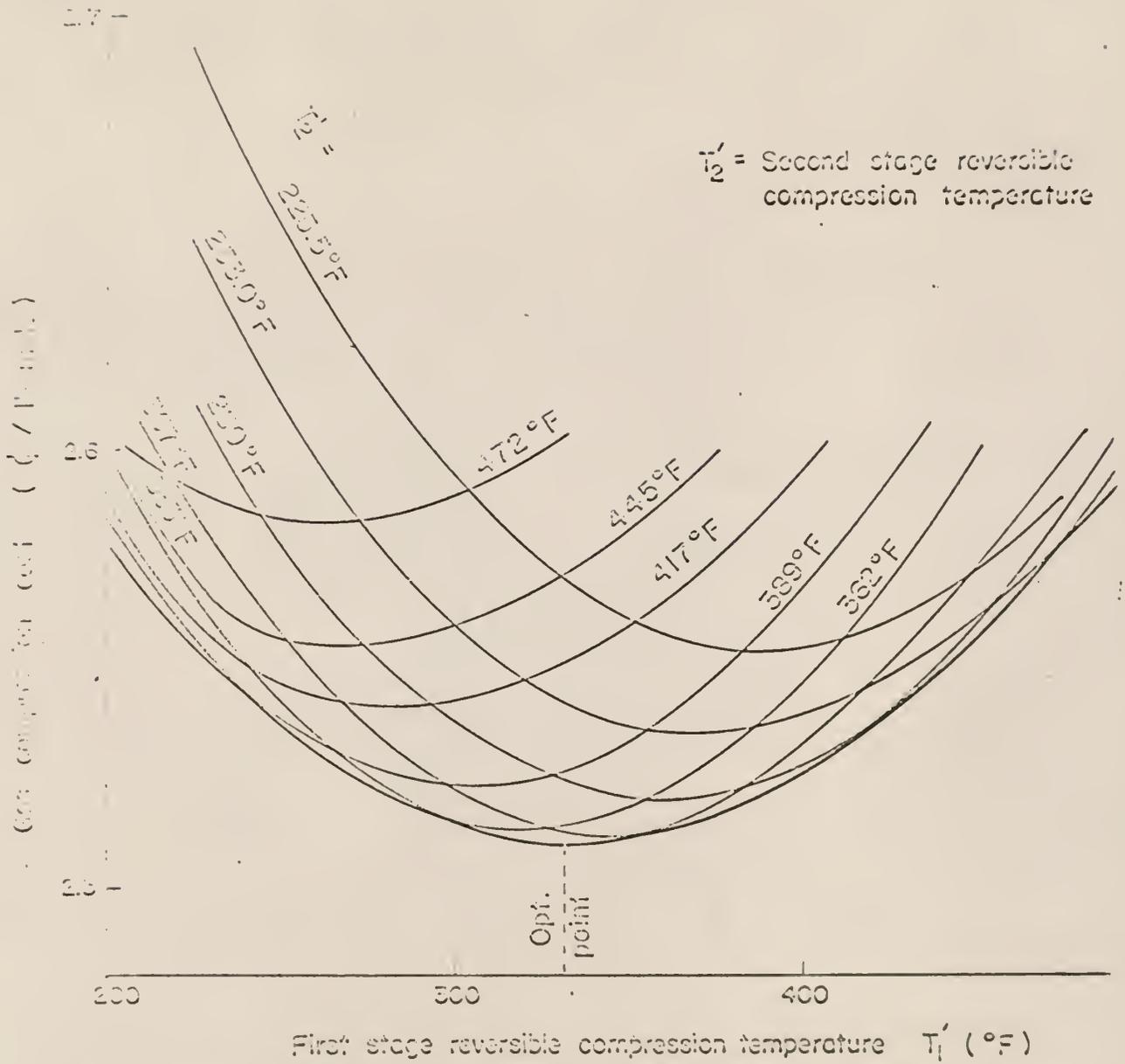


Fig. 10. Gas compression cost for CO_2 gas in two dimensional problems with the first and second stage reversible compression temperatures as the control variables.

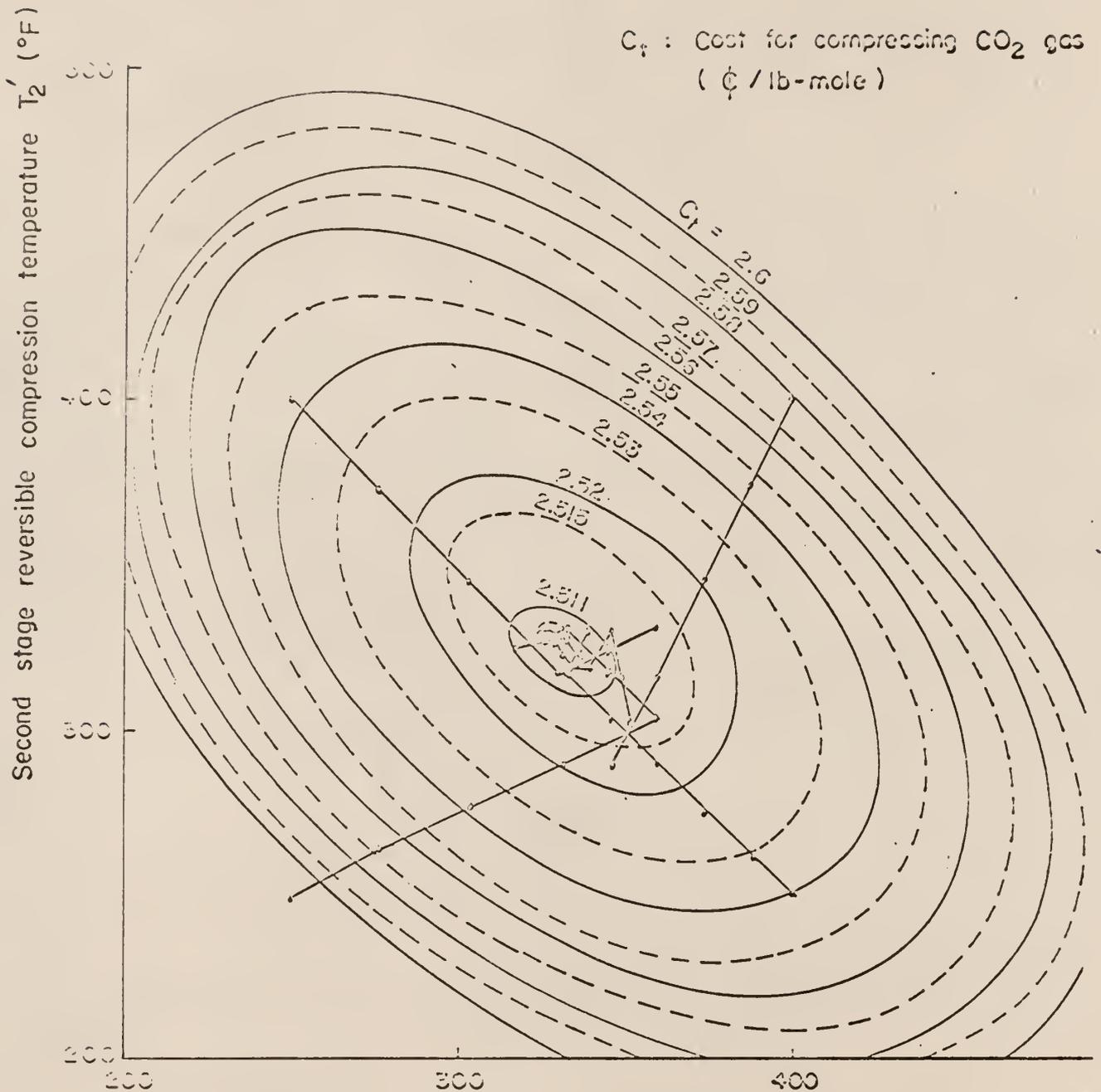


Fig. 1. First stage reversible compression temperature T_1' (°F) vs. second stage reversible compression temperature T_2' (°F) and compression cost for CO_2 gas in two dimensional problems with the first and second stage reversible compression temperatures as control variables.

Numerical values of the constants in the performance equations are summarized in Table 4. Find the optimum conditions for all the problems and also find the costs under the optimum conditions.

These problems have been solved and the results are summarized by Figures 12-20.

Figure 12 summarizes how the intermediate stage pressures P_1 and P_2 (—lines) vary with the discharge temperature at the discharge pressure of 500 Psi. The optimum intermediate pressures as calculated by the conventional ideal gas assumption are also shown (--- lines) for comparison. Figures 13, 14, 15 and 16 similarly show the optimum intermediate stage pressures under discharge pressures of 800, 1100, 1400 and 1700 psi respectively. By reviewing the figures, it will be seen that the differences in the optimum intermediate stage pressures increase as the discharge pressure increases.

Figures 17A and 17B respectively show how the optimum first stage pressure and second stage pressure vary with discharge temperature under various discharge pressures. Figure 18 shows how the optimum intermediate stage temperature after hypothetical reversible compression varies with the discharge pressure under various discharge pressures as calculated by the present method.

Figure 19 shows how the gas compression cost under optimum conditions as calculated by the present method varies with the discharge temperature under various discharge pressures. In the figure, gas compression cost under the optimum condition as calculated by the conventional approach is also shown for comparison. It shows that

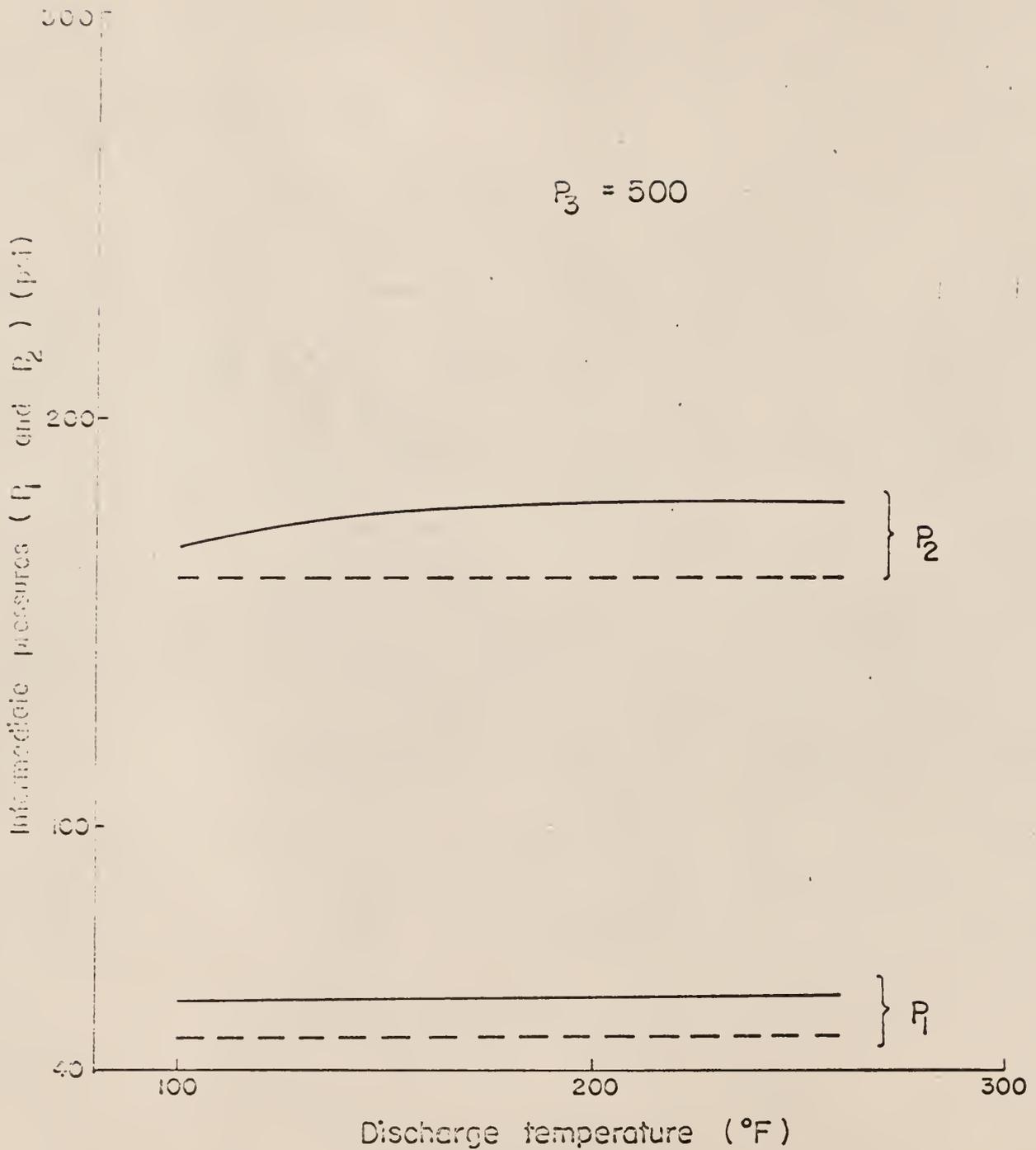


Fig. 12. Optimal intermediate pressures, P_1 and P_2 , vs. discharge temperature T_3 as calculated by the conventional ideal gas approach (---) and the present approach (—) at $P_3 = 500$ psi.

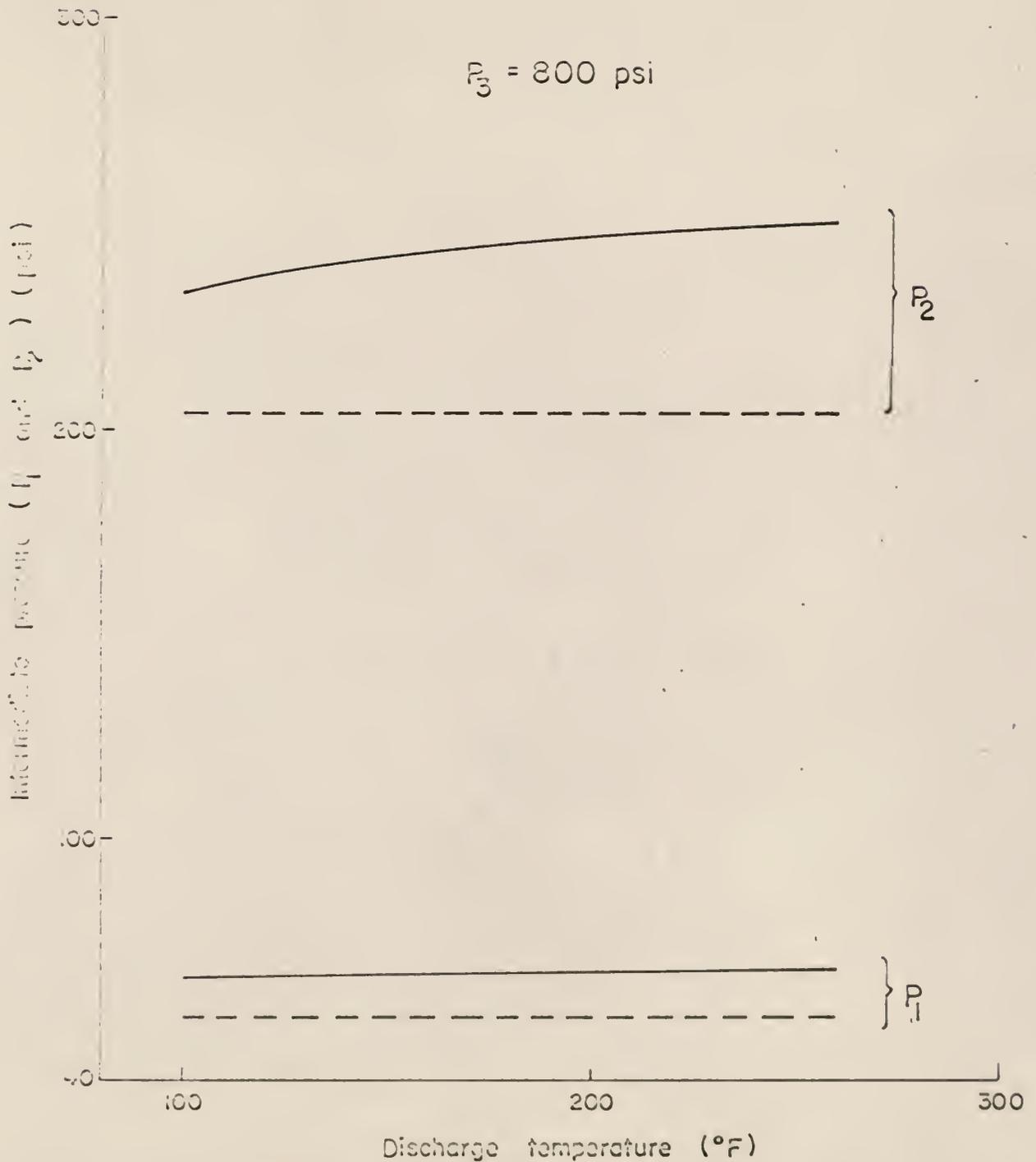


Fig. 13. Optimal intermediate pressure P_1 and P_2 vs. discharge temperature T_3 as calculated by the conventional ideal gas approach (---) and the present approach (—) at $P_3 = 800 \text{ psi}$.

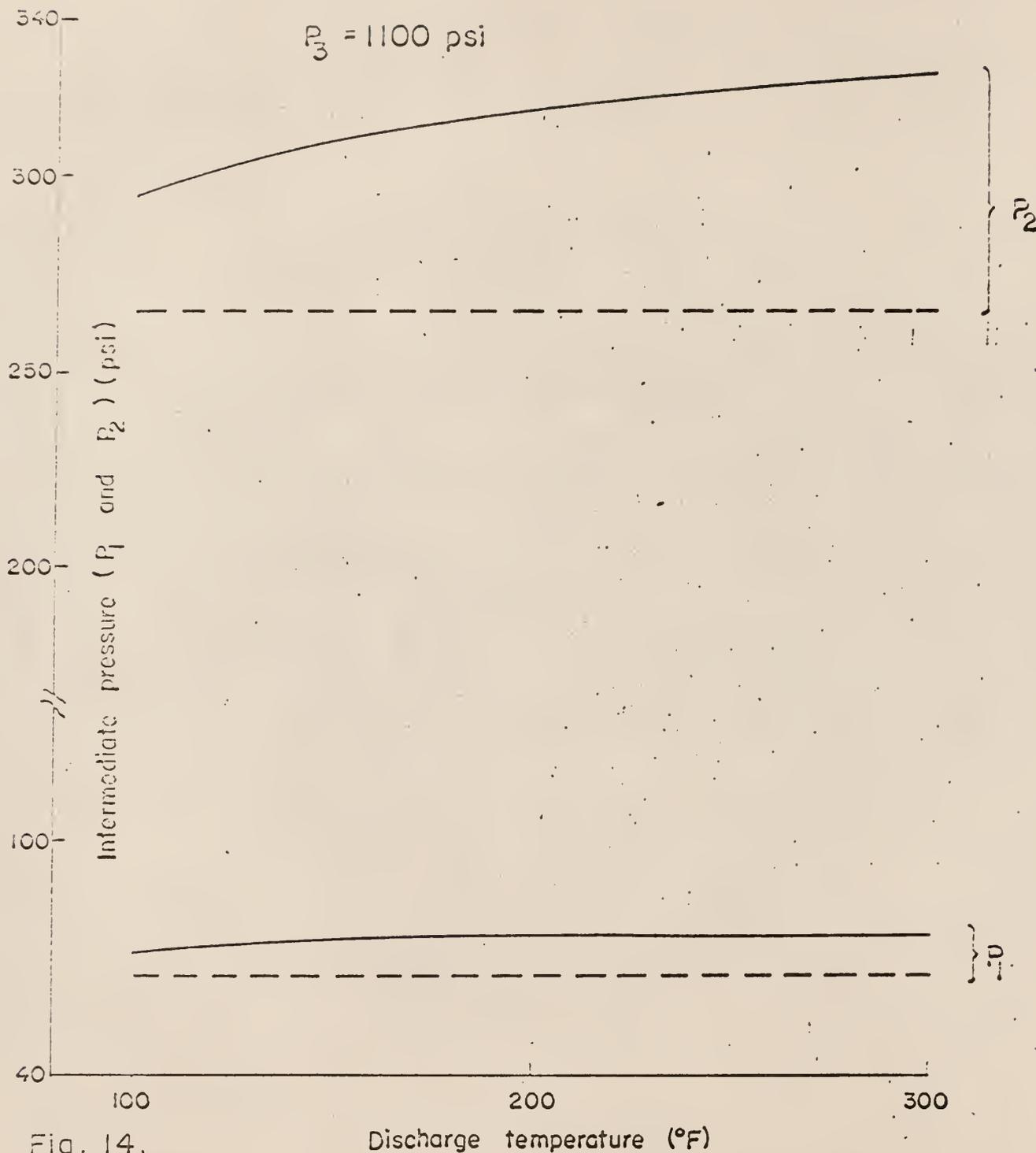


Fig. 14.

Discharge temperature ($^{\circ}F$)

Optimal intermediate pressure P_1 and P_2 vs. discharge temperature T_3 as calculated by the conventional ideal gas approach (---) and the present approach (—) at $P_3 = 1100$ psi.

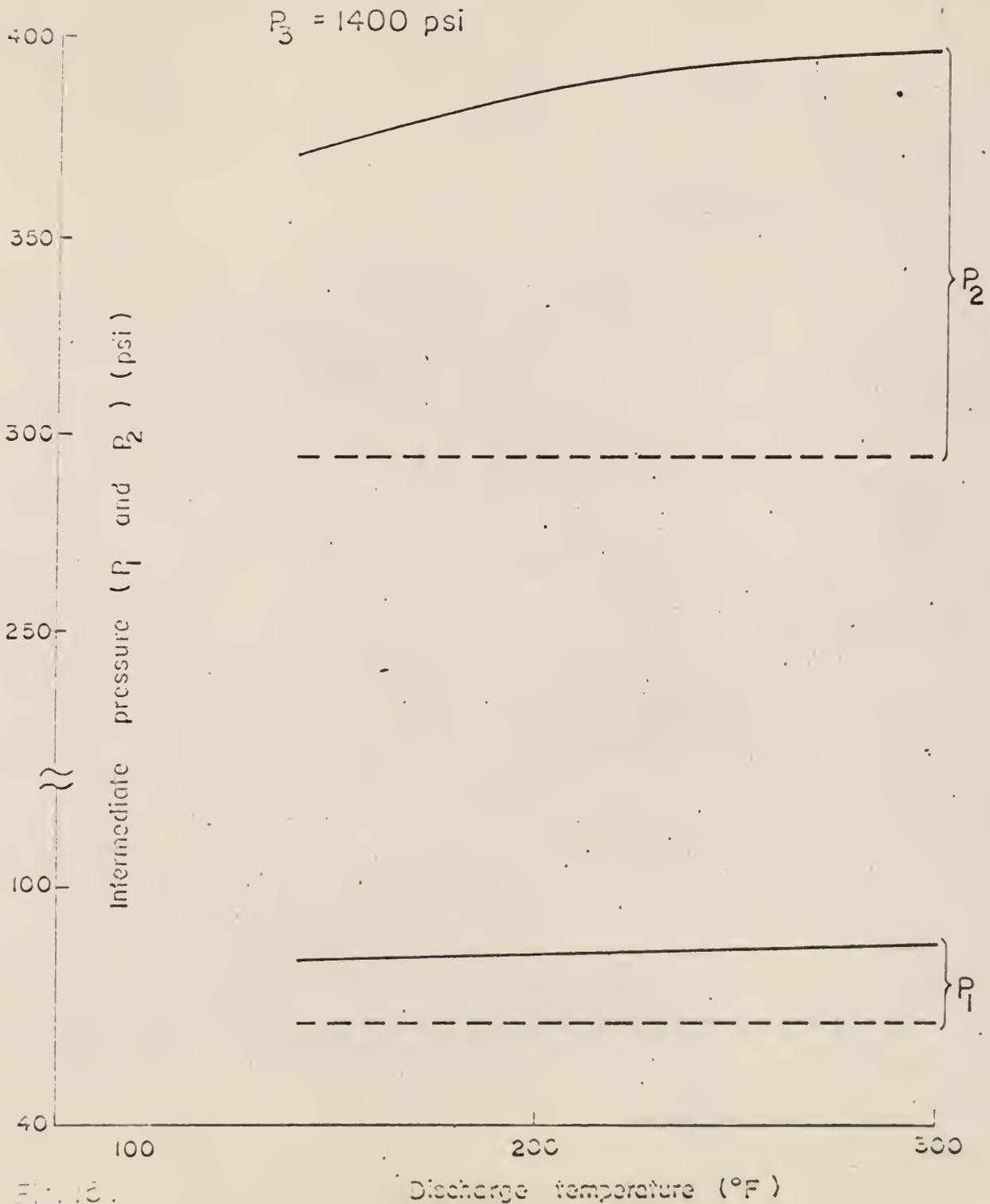


Fig. 18.

Optimal intermediate pressure P_1 and P_2 vs. discharge temperature T_3 as calculated by the conventional ideal gas approach (---) and the present approach (—) at $P_3 = 1400 \text{ psi}$.

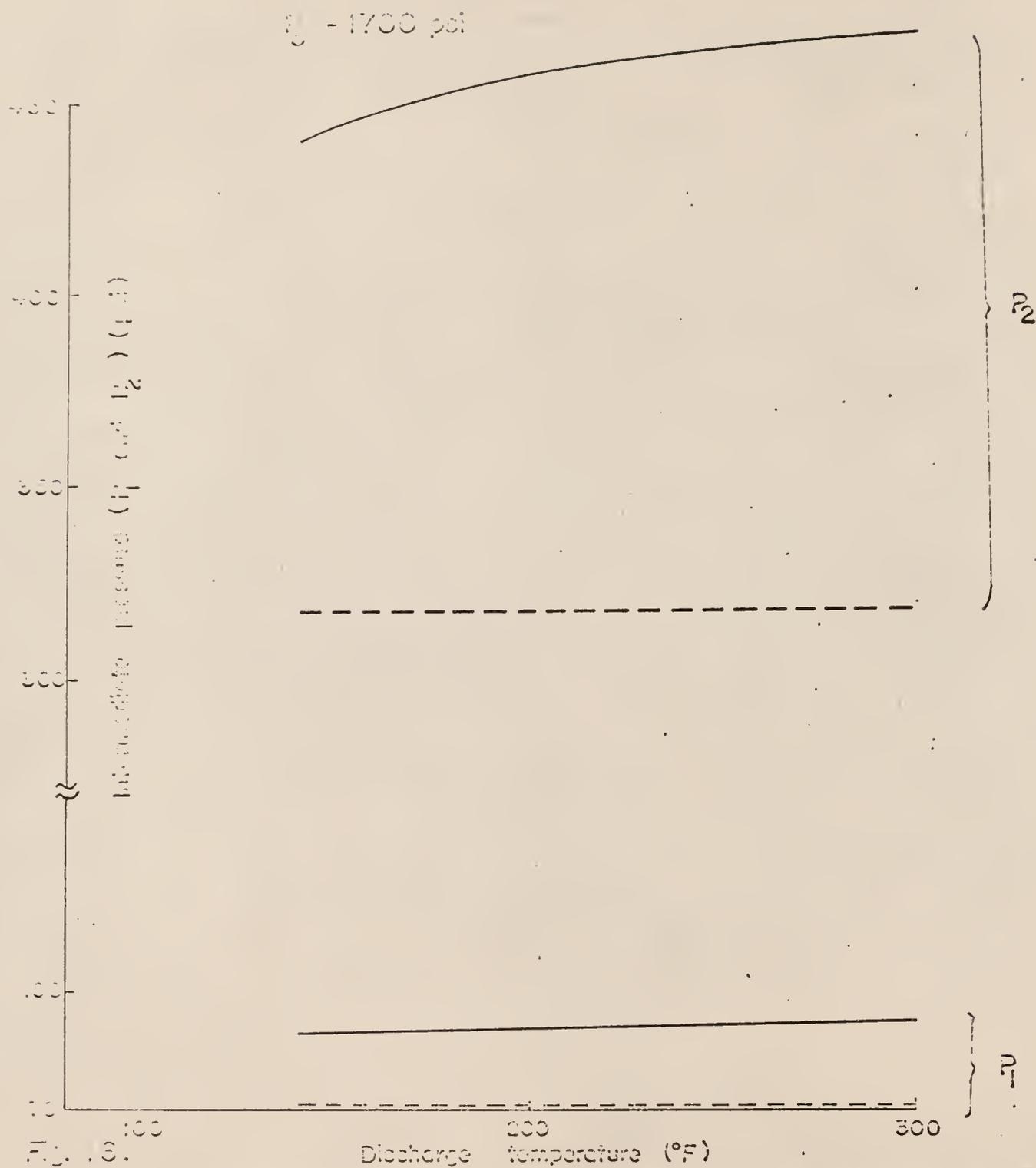


Fig. 16.

Optimal intermediate pressure P_1 and P_2 vs. discharge temperature T_3 as calculated by the conventional ideal gas approach (---) and the present approach (—) at $P_3 = 1700 \text{ psi}$.

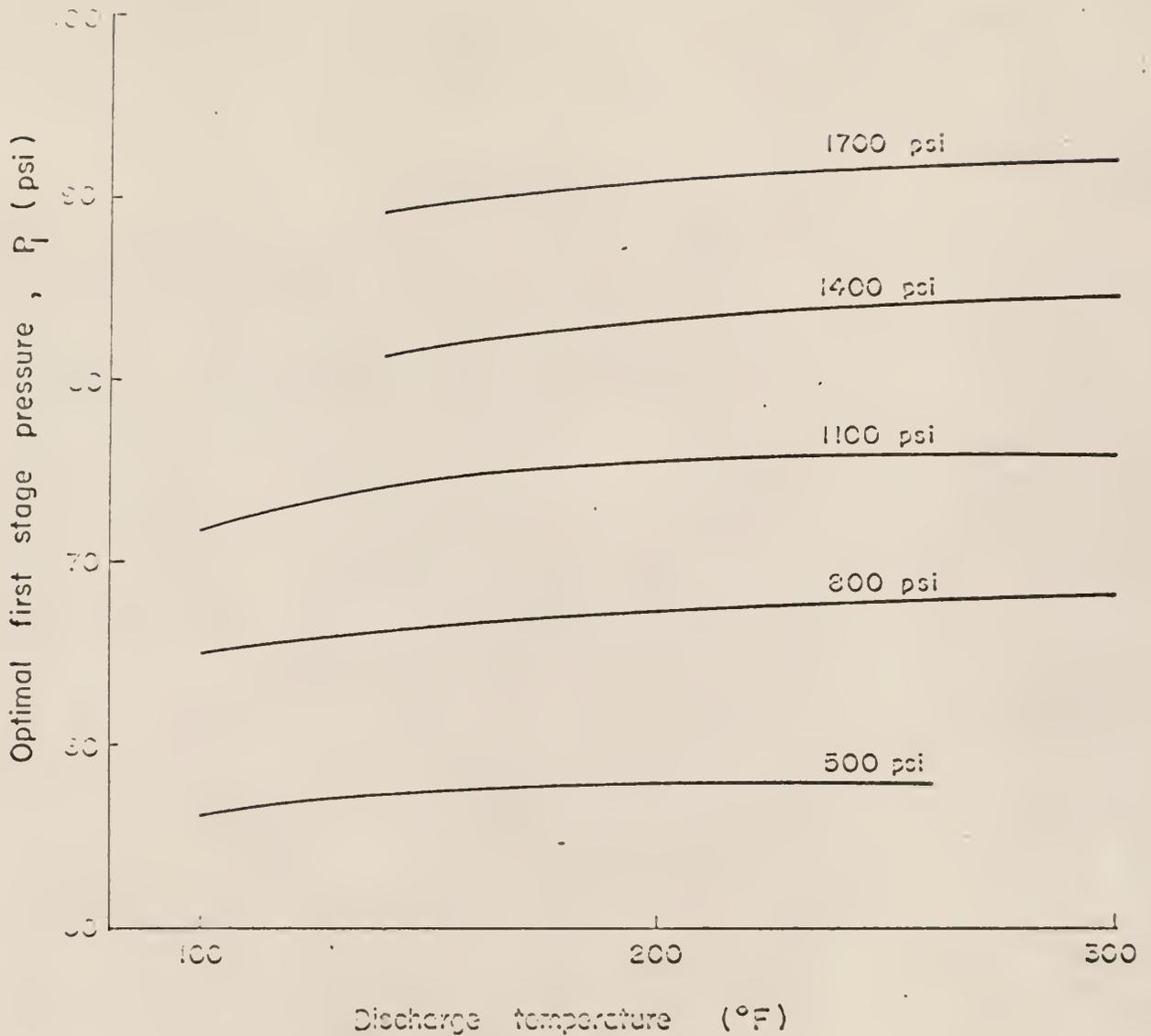


Fig. 17-2. Optimal first stage pressure P_1 vs. discharge temperature T_3 at various discharge pressure P_3 for a three-stage gas compression of CO_2 gas.

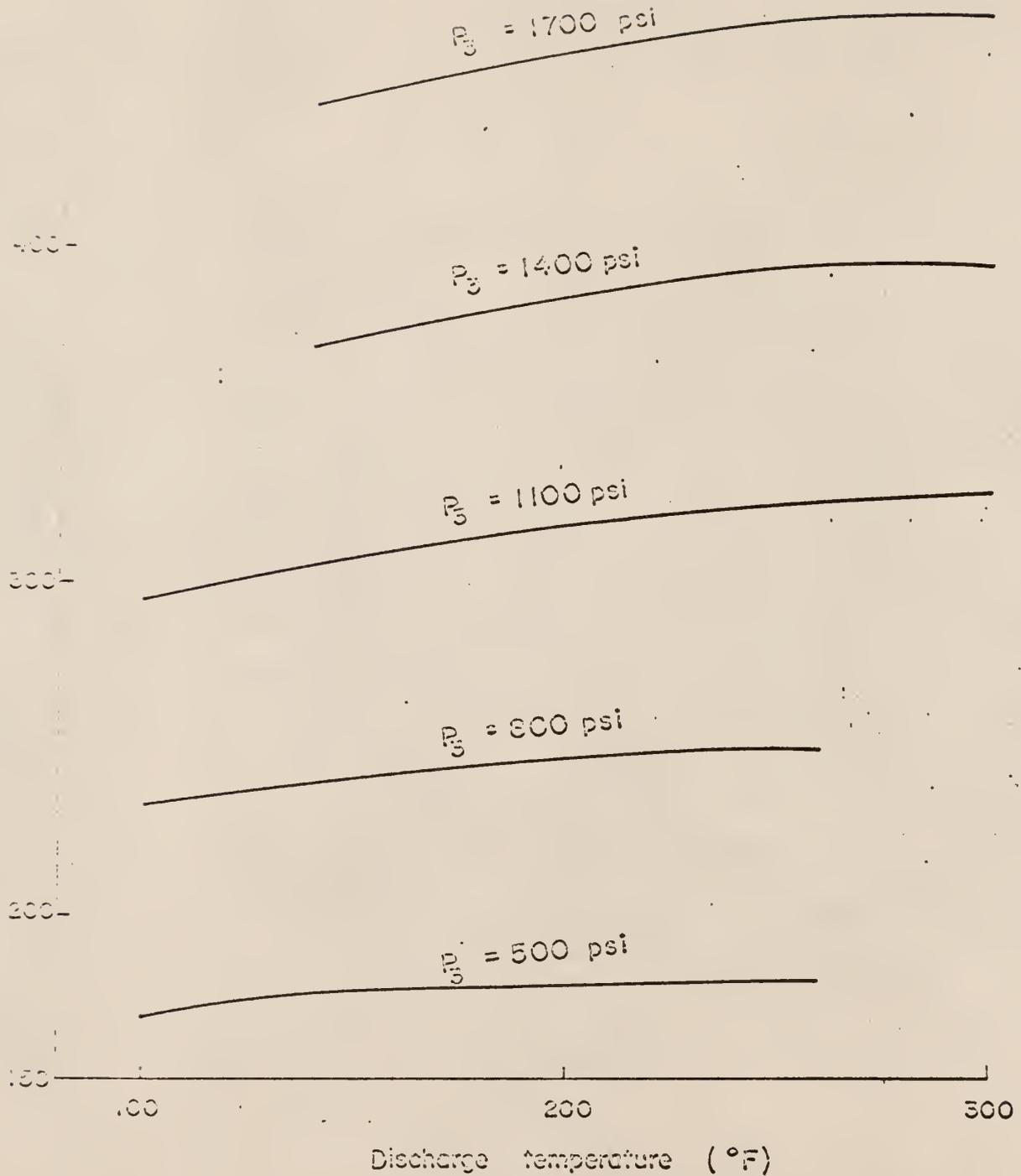
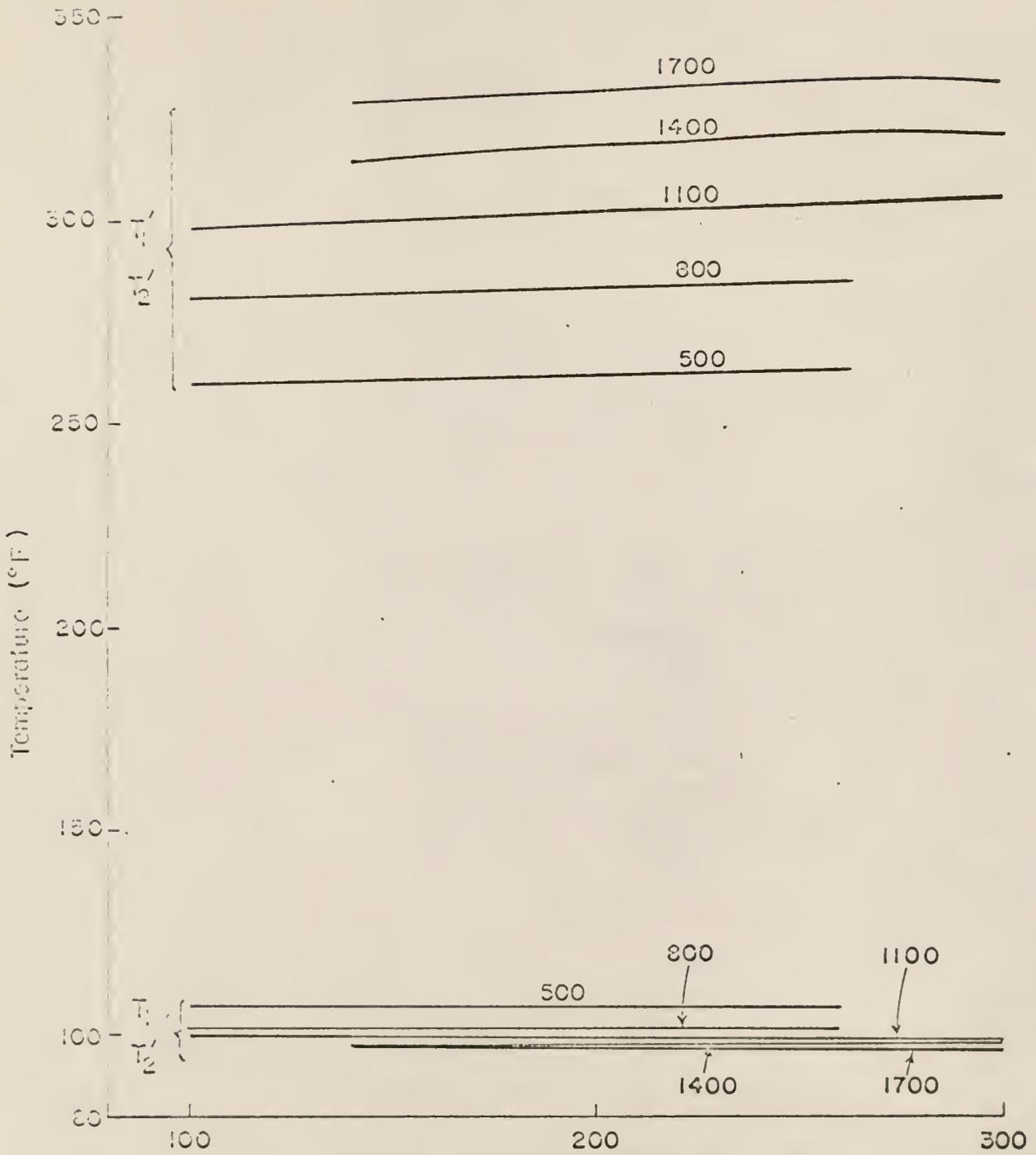


Fig. 7-8-Optimal second stage pressure P_2 vs. discharge temperature T_2 at various discharge pressure P_3 for three-stage gas compression of CO_2 gas.



T_3 : Discharge temperature from the third stage (°F)

Fig. 13. Temperature after reversible compressions and after interstage coolings .

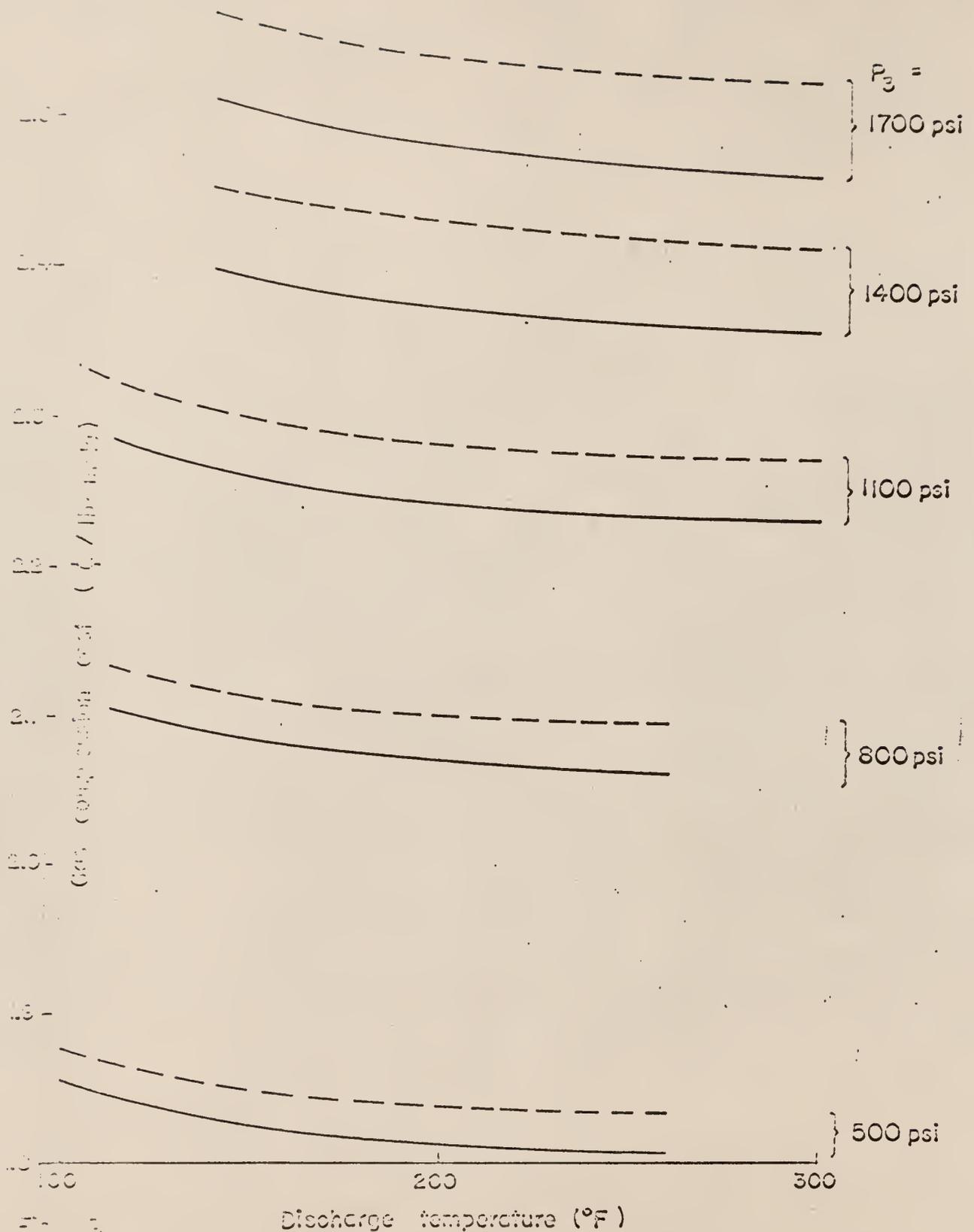


Fig. 13.

Discharge temperature (°F)

Comparison of the optimum gas compression (CO₂, three stages) costs as calculated by the conventional ideal gas approach (---) and the present approach (—).

significant cost saving can be obtained if the gas compression is conducted under the optimum condition as calculated by the present method. Figure 20 shows the % cost reduction in gas compression cost obtainable if gas compression is conducted under the optimum policy calculated by the present method as compared with the case where the optimum policy is calculated by the conventional ideal gas method. It shows that the % cost reduction increases as the discharge pressure increases and the cost saving obtainable is fairly significant. For example, a 2.5% cost saving is realizable by operating under the optimum condition calculated by the present study as compared with the case when the optimum policy is calculated by the conventional approach.

Figure 21 shows the computer flow diagram used in the programming, and Table 6 shows the computer program used to obtain the numerical results described above.

IV. SUMMARY

The optimization technique developed in this study is based on the discrete analog of the maximum principle and an iterative search method. The technique employs four Lagrange multipliers in each stage in association with the four equality constraints. The method is fairly general and can be used in conjunction with any equation of state.

The equation of state developed by Hirshfelder et al. is used in deriving the performance equations. Numerical computations have been made for several problems related to 3-stage gas compression

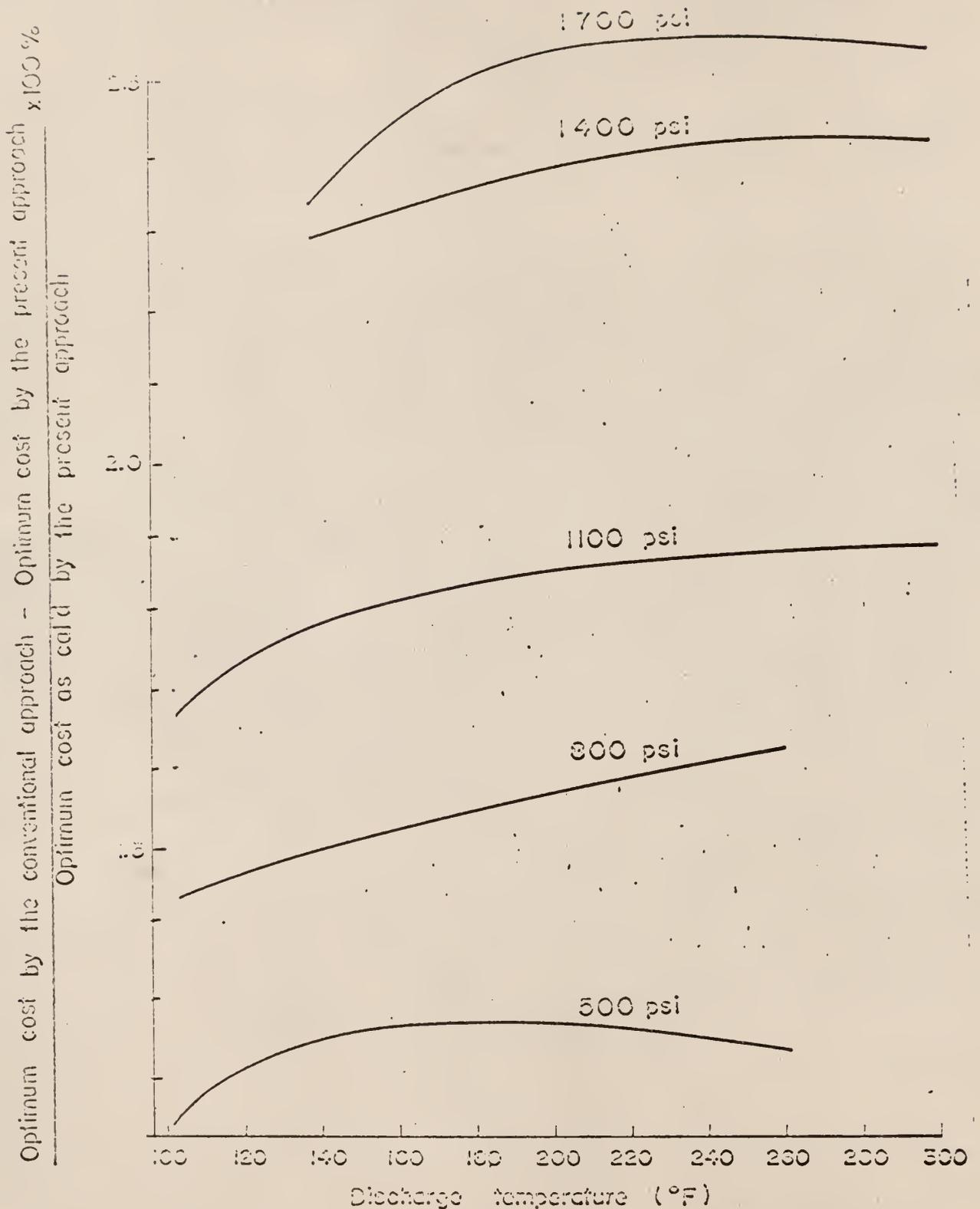


FIG. 20. % reduction in optimum cost vs. discharge temperature at various discharge pressures for three-stage gas compression of CO_2 gas by the present approach as compared with the conventional approach.

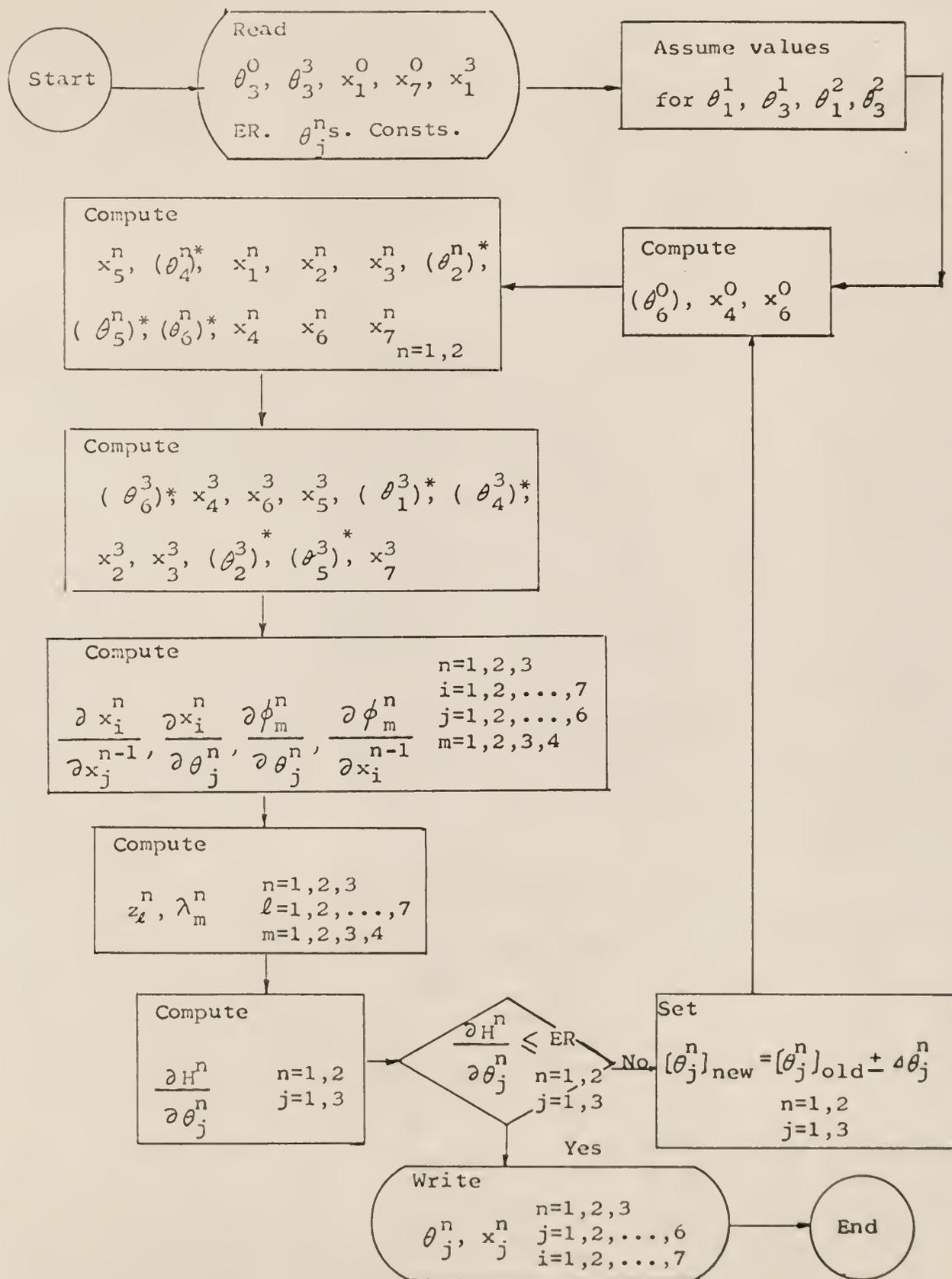


Fig. 21. Computer flow diagram

*Values to be obtained by iteration.

of carbon dioxide gas within region I. The computational scheme developed here can be applied to any gas under a rather wide range of temperature and pressure. The numerical computations have given rise to the following significant results:

1. The optimal policy of a multistage gas compression system is affected not only by the discharge pressure but also by the discharge temperature. For example, Fig. 15 shows that the optimum second stage pressure for a three-stage CO₂ gas compression system discharging at 1400 psia varies from 370 psia to 400 psia as the discharge temperature varies from 120 °F to 300 °F.
2. The optimal policy of a three-stage carbon dioxide gas compression system as computed by the present approach is significantly different from the policy as computed by the conventional approaches. For example, at the discharge pressure of 1400 psia and discharge temperature of 300 °F, the optimum first and second stage pressures as computed by the present approach are 86 psia and 400 psia respectively. The optimal first and second stage pressures computed by the conventional approaches are 56 psia and 296 psia respectively.
3. The gas compression cost evaluated by the present approach at the optimum condition is significantly lower than the gas compression cost evaluated at the optimum condition as determined by the conventional approach. The difference in these costs is summarized in Figure 19. It is shown that the cost difference increase as the discharge pressure increases.

Figure 20 shows % cost saving as a function of discharge tem-

perature and pressure. The cost saving is about 2.5% for CO₂ compression at the discharge pressure of 1700 psia.

All the numerical computation has been made by IBM 360 computer. Computing time for one iteration as described in section IV of Chapter 5 is 20 seconds. Assuming that 15 iterations are required to arrive at the optimum policy, the computing time required is 5 minutes for solving an optimization problem considered in this work.

Nomenclature

- A_n = heat transfer area of the n-th stage intercooler, ft^2
 b = a constant appearing in the equation of state; 0.1985
 for CO_2
 b' = a constant appearing in the equation of state; 0.739
 for CO_2
 C_e = unit power cost; 2.94×10^{-6} \$/Btu.
 C_H = capital cost per unit heat transfer area; 7 \$/ft²
 C_{HP} = capital cost for compressors per HP; 100 \$/HP =
 3.93×10^{-2} \$/Btu/hr
 C_p = heat capacity of CO_2 gas per lb-mol, Btu/lb-mol °R:

$$C_p = 16.2 - \frac{6.53 \times 10^3}{T} + \frac{1.41 \times 10^6}{T^2} \quad (\text{Ref. 21})$$

 $(C_p)_w$ = heat capacity of cooling water; 1 Btu/lb °R
 C_w = unit cooling water cost; 1.5×10^{-6} \$/lb
 E_1^n = cost due to the power consumed in the n-th stage
 compressor, \$/lb-mole.
 E_2^n = cost due to allocating the initial cost of the n-th
 stage compressor, \$/lb-mole
 E_3^n = cost due to allocating the initial cost of the n-th
 stage heat exchanger, \$/lb-mole
 E_4^n = cost due to the cooling water used in the n-th
 stage intercooler, \$/lb-mole
 H = enthalpy of gas, Btu/lb-mol
 H_n = enthalpy of the gas leaving the n-th stage intercooler
 Btu/lb-mole

H'_n = enthalpy of the gas after the n-th stage reversible compression, Btu/lb-mole

H''_n = enthalpy of the gas after n-th stage actual compression, Btu/lb-mole

H_0 = enthalpy of the gas at hypothetical ideal gas state at the temperature of the gas, Btu/lb-mole

H^0 = enthalpy of the gas at hypothetical ideal gas state and at a reference temperature T_0 , Btu/lb-mole

H^n = Hamiltonian function at n-th stage

H^N = Hamiltonian function at the last stage

k_0 = a constant appearing in the equation of state; 5.5

k_1 = a constant appearing in the equation of state; 1.43

k_2 = a constant appearing in the equation of state; 1.33

k_3 = a constant appearing in the equation of state; 1.478

k_4 = a constant appearing in the equation of state; 0.794

m = flow rate, lb-moles/hr

N = total number of stage

P = pressure of the gas, psi

P_0 = pressure of the gas at inlet condition, psi

pressure of the gas at the standard condition, psi

P_c = critical pressure of the gas, psi

p = reduced pressure of the gas, $p = \frac{P}{P_c}$

P_n = pressure of the gas at the n-th stage, dimensionless

R = gas law constant; $1.98 \frac{\text{Btu}}{\text{lb-mole } ^\circ\text{R}}$

S = entropy of the gas, Btu/lb-mole $^\circ\text{R}$

- s_n' = entropy of the gas after the hypothetical reversible compression at n-th stage, Btu/lb-mole $^{\circ}\text{R}$.
- S_0' = entropy of the gas under hypothetical ideal gas state at the temperature of the gas and at the critical pressure of the gas, Btu/lb-mole R
- S_2^* = entropy of the gas under the hypothetical ideal gas state at the temperature of the gas and occupying the same volume as the actual gas, Btu/lb-mole $^{\circ}\text{R}$
- S_0 = entropy of the gas at a hypothetical ideal gas state and at the standard pressure, Btu/lb-mole $^{\circ}\text{R}$
- T = absolute temperature of the gas $^{\circ}\text{R}$
- T_0 = absolute temperature of the reference state, $^{\circ}\text{R}$
- T_c = critical temperature of the gas, $^{\circ}\text{R}$
- t = reduced temperature of the gas, $t = \frac{T}{T_c}$
- t_n = reduced temperature of the gas leaving the n-th stage intercooler
- t_n' = reduced temperature of the gas after n-th stage reversible compression
- t_n'' = reduced temperature of the gas after n-th stage actual compression
- $(t_w)_i$ = ratio of the absolute temperature of cooling water entering the coolers over the critical temperature of the gas
- $(t_w)_o$ = ratio of the absolute temperature of cooling water leaving the coolers over the critical temperature of the gas

- U = overall coefficient of heat transfer in the intercoolers; 5 Btu/ft²/hr. °R
- V = volume of the gas; cu-ft/lb-mole
- V_c = critical volume of the gas; cu-ft/lb-mole
- V_o' = volume of the gas under a hypothetical ideal gas state at the temperature of the gas and at the critical pressure of the gas
- x_i^n = a state variable
- z_c = compressibility of the gas at critical condition; for CO₂ gas 0.275
- z_i^n = adjoint variable associated with x_i^n
- ρ = reduced density of the gas; $= \frac{V_c}{V}$
- ρ_n = reduced density of the gas leaving the n-th stage cooler
- ρ_n' = reduced density of the gas after n-th stage reversible compression
- ρ_n'' = reduced density of the gas after n-th stage actual compression
- ψ_1, ψ_2 = fractions of the initial cost of a gas compressor and an intercooler allocated and chargeable to an hour operation respectively: in the numerical computations they are assumed to be the same and taken as 9.4×10^{-6} .
- ϕ_i^n = constraint functions at n-th stage

Table 5. Definition of Computer Notations

<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>	<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>
AH	H^0	DHT	$\Delta\theta_2^n$
AKO	k_0	DIT	$\Delta\theta_6^n$
AK1	k_1	DJT	$\Delta\theta_1^n$
AK2	k_2	DKT	$\Delta\theta_1^n$
AK3	k_3	DLT	$\Delta\theta_3^n$
AK4	k_4		
ALM1(n+1)	λ_1^n	HTI(n+1)	$\frac{\partial H^n}{\partial \theta_1^n}$
ALM2(n+1)	λ_2^n	HT3(n+1)	$\frac{\partial H^n}{\partial \theta_3^n}$
ALM3(n+1)	λ_3^n	P1T1(n+1)	$\frac{\partial \phi_1^n}{\partial \theta_1^n}$
ALM4(n+1)	λ_4^n		
AS	S^0	P1T2(n+1)	$\frac{\partial \phi_1^n}{\partial \theta_2^n}$
B1	b	P1T4(n+1)	$\frac{\partial \phi_1^n}{\partial \theta_4^n}$
B2	b'		
CE	C_e	P1T5(n+1)	$\frac{\partial \phi_1^n}{\partial \theta_5^n}$
CH	C_H	P2T1(n+1)	$\frac{\partial \phi_2^n}{\partial \theta_1^n}$
CHP	C_{HP}		
CPW	$(C_p)_w$	P2T3(n+1)	$\frac{\partial \phi_2^n}{\partial \theta_3^n}$
CW	C_w		
CZ	Z_c	P2T4(n+1)	$\frac{\partial \phi_2^n}{\partial \theta_4^n}$
DET	$\Delta\theta_6^n$	P2T6(n+1)	$\frac{\partial \phi_2^n}{\partial \theta_6^n}$
DFT	$\Delta\theta_4^n$		
DGT	$\Delta\theta_5^n$		

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Chapter 5

Table 5. Definition of Computer Notations--Continued

<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>	<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>
P3T1(n+1)	$\frac{\partial \phi_3^n}{\partial \theta_1^n}$	POC	$\frac{P_o}{P_c}$
		R	R
P3T4(n+1)	$\frac{\partial \phi_3^n}{\partial \theta_4^n}$	T1(n+1)	θ_1^n, t_n'
		T2(n+1)	θ_2^n, t_n''
P3T6(n+1)	$\frac{\partial \phi_3^n}{\partial \theta_6^{n-1}}$	T3(n+1)	θ_3^n, t_n
		T4(n+1)	θ_4^n, t_n'
P4T1(n+1)	$\frac{\partial \phi_4^n}{\partial \theta_1^n}$	T5(n+1)	θ_5^n, t_n''
		T6(n+1)	θ_6^n, t_n
P4T2(n+1)	$\frac{\partial \phi_4^n}{\partial \theta_2^n}$	T1P(n+1)	θ_1^n in memory
		T3P(n+1)	θ_3^n in memory
P4T4(n+1)	$\frac{\partial \phi_4^n}{\partial \theta_4^n}$	TC	T_c
		TO	t_o
P4T5(n+1)	$\frac{\partial \phi_4^n}{\partial \theta_5^n}$	TWI	$(t_w)_i$
		TWO	$(t_w)_o$
P4X4(n+1)	$\frac{\partial \phi_4^n}{\partial x_4^{n-1}}$	U	U
		X1(n+1)	x_1^n, P_n, P_n', P_n''
PH	ψ_1, ψ_2	X2(n+1)	x_2^n, H_n'

Table 5. Definition of Computer Notations--Continued

<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>	<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>
X3(n+1)	x_3^n, H_n''	X3T2(n+1)	$\frac{\partial x_3^n}{\partial \theta_2^n}$
X4(n+1)	x_4^n, H_n		
X5(n+1)	x_5^n, S_n'	X3T5(n+1)	$\frac{\partial x_3^n}{\partial \theta_5^n}$
X6(n+1)	x_6^n, S_n		
X7(n+1)	x_7^n, C_n	X4T3(n+1)	$\frac{\partial x_4^n}{\partial \theta_3^n}$
X1T1(n+1)	$\frac{\partial x_1^n}{\partial \theta_1^n}$		
X1T2(n+1)	$\frac{\partial x_1^n}{\partial \theta_2^n}$	X4T6(n+1)	$\frac{\partial x_4^n}{\partial \theta_6^n}$
X1T3(n+1)	$\frac{\partial x_1^n}{\partial \theta_3^n}$	X5T1(n+1)	$\frac{\partial x_5^n}{\partial \theta_1^n}$
X1T4(n+1)	$\frac{\partial x_1^n}{\partial \theta_4^n}$	X5T4(n+1)	$\frac{\partial x_5^n}{\partial \theta_4^n}$
X1T5(n+1)	$\frac{\partial x_1^n}{\partial \theta_5^n}$	X6T3(n+1)	$\frac{\partial x_6^n}{\partial \theta_3^n}$
X1T6(n+1)	$\frac{\partial x_1^n}{\partial \theta_6^n}$	X6T6(n+1)	$\frac{\partial x_6^n}{\partial \theta_6^n}$
X2T1(n+1)	$\frac{\partial x_2^n}{\partial \theta_2^n}$	X7T2(n+1)	$\frac{\partial x_7^n}{\partial \theta_2^n}$
X2T4(n+1)	$\frac{\partial x_2^n}{\partial \theta_4^n}$		

Table 5. Definition of Computer Notations--Continued

<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>	<u>Computer notation</u>	<u>Conventional and/or maximum principle notation</u>
X7T3(n+1)	$\frac{\partial x_7^n}{\partial \theta_3^n}$	Z1(n+1)	z_1^n
		Z2(n+1)	z_2^n
X7T5(n+1)	$\frac{\partial x_7^n}{\partial \theta_5^n}$	Z3(n+1)	z_3^n
		Z4(n+1)	z_4^n
		Z5(n+1)	z_5^n
X7T6(n+1)	$\frac{\partial x_7^n}{\partial \theta_6^n}$	Z6(n+1)	z_6^n
		Z7(n+1)	z_7^n
X7X4(n+1)	$\frac{\partial x_7^n}{\partial x_4^{n-1}}$		
X7X7(n+1)	$\frac{\partial x_7^n}{\partial x_7^{n-1}}$		

Table 6. Computer Program

```

C      COST OPTIMIZATION OF PUMP SYSTEM
      DIMENSION T1(4),T2(4),T3(4),T4(4),T5(4),T6(4),X1(4),X2(4),X3(4)
      DIMENSION X4(4),X5(4),X6(4),X7(4),X1T1(4),X1T4(4),X2T1(4),X2T4(4)
      DIMENSION X3T2(4),X3T5(4),X4T5(4),X4T3(4),X4T6(4),X5T1(4),X5T4(4)
      DIMENSION X6T3(4),X6T6(4),X7T2(4),X7T3(4),X7T6(4),X7X4(4)
      DIMENSION X7X7(4),P1T1(4),P1T2(4),P1T4(4),P1T5(4),P2T1(4)
      DIMENSION P2T3(4),P2T4(4),P2T6(4),P3T1(4),P3T4(4),P3X6(4),P4T1(4)
      DIMENSION P4T2(4),P4T4(4),P4T5(4),P4X4(4),DKT(4),DLT(4),T1P(4)
      DIMENSION Z1(4),Z2(4),Z3(4),Z4(4),Z5(4),Z6(4),Z7(4),ALM1(4)
      DIMENSION ALM2(4),ALM3(4),ALM4(4),HT1(3),HT3(3),X7T5(4),T3P(4)
1001  FORMAT(8E10.4)
1002  FORMAT(7F16.8)
      READ(1,1001) AKO,AK1,AK2,AK3,AK4,B1,B2
      READ(1,1001) POC,CZ,R,TC
      READ(1,1001) TWO,TWI,TO,CHP,CH,PH,CW,CPW
      READ(1,1001) AH,AS,U,CE
      READ(1,1001) T3(1),X1(1),X7(1)
      N=0
1      N=N+1
      IF(N.EQ.3) GO TO 520
      READ(1,1001) X1(4)
      M=0
2      M=M+1
      IF(M.EQ.6) GO TO 510
      READ(1,1001) T3(4)
      READ(1,1001) T1(2),T3(2),T1(3),T3(3)
      READ(1,1001) HT1(2),HT3(2),T1P(2),T3P(2)
      READ(1,1001) HT1(3),HT3(3),T1P(3),T3P(3)
      READ(1,1001) DKT(2),DKT(3),DLT(2),DLT(3)
      L=0
4      L=L+1
      IF(L.EQ.16) GO TO 500
      READ(1,1001) DET,DFT,DGT,DHT,DIT,DJT
      READ(1,1001) T4(2),T5(2),T6(2),T2(2)
      READ(1,1001) T4(3),T5(3),T6(3),T2(3)
      READ(1,1001) T4(4),T5(4),T6(4),T2(4),T1(4)
      DX5=1.
      I=1
5      DX1=1.
10     XIC = -(AKO+AK1/T3(I))(T6(I)**2.+AK2*(-T3(I)+1./T3(I))*T6(I)**3.
      1+T6(I)*T3(I)/(CZ*(1.-B1*T6(I)+B2*T6(I)*T6(I)))
      DX1P=DX1
      DX1=X1(I)-X1C
      IF(ABS (DX1)-AB)80,80,30
30     IF(DX1P*DX1) 40,40,50
40     DFT=DET/2.
50     IF(DX1)60,60,70
60     T6(I)=T6(I)-DET
      CO TO 10
70     18(I)=T6(I)+DET
      GO TO 10

```

```

80      CONTINUE
      TT=ALOG(T3(I)*TC/TO)
      TT1=1./((T3(I)*TC)-1./TO)
      TCP1=16.2*(T3(I)*TC-TO)-3530.*TT-1410000.*TT1
      TCS1=16.2*TT+6530.*TT1-705000.*(1./((T3(I)*TC)**2.-1./TO**2.))
      X4(I)=-CZ*R*TC*T3(I)*(T6(I)I(2.*AKO/T3(I)+3.*AK1/T3(I)**2.))-
      1CZ*R*TC*T3(I)*(AK2*T6(I)*16(I)*(1.-2./T3(I)**2.))+R*TC*T3(I)*B1*
      2T6(I)-B2*T6(I)*T6(I))/(1.-B1*T6(I)+B2*T6(I)*T6(I))+AH+TCP1
      X6(I)=R*(CZ*(-AK1*T6(I)/T3(I)**2.+0.5*AK2*T6(I)*T6(I)*(1.-
      11./T3(I)**2.))-ALOG(T6(I)*T3(I))+0.5*ALOG(1.-B1*T6(I)+
      2B2*T6(I)*T6(I))-AK3*ATAN (AK3)-AK3*ATAN (AK4*T6(I)-AK3)+ALOG(CZ))+
      3R*ALOG(PCC)+A5+TCS1
      KRITE(3,1002) T3(I),T6(1)
      KRITE(3,1002) X1(1),X4(I),X6(I),X7(I)
      IF(I.FQ.4) GO TO 100
      DG 300 I=2,3
100     READ(1,1001) DET,DFT,DCT,DHT,DIT
      X5(I)=X6(1-1)
      IF(I.FO.4) GO TO 305
      TT1=1./((T1(I)*TC)-1./TO)
      TT=ALOG(T1(I)*TC/TO)
      TCP2=16.2*(T1(I)*TC-TO)-6530.*TT-1410000.*TT1
      TCS2=16.2*TT+6530.*TT1-705000.*(1./((T1(I)*TC)**2.-1./TO**2.))
      DX1=1.
110     X5C = R*(CZ*(-AK1*T4(I)/T1(I)**2.+0.5*AK2*T4(I)*T4(I)*(1.-
      11./T1(I)**2.))-ALOG(T4(I)*T1(I))+0.5*ALOG(1.-B1*T4(I)+
      2B2*T4(I)*T4(I))-AK3*ATAN (AK3)-AK3*ATAN (AK4*T4(I)-AK3)+ALOG(CZ))+
      3R*ALOG(POC+AS+TCS2)
      DX1P=DX1
      DX1=X5(I)-X5C
      IF(ABS(DX)-AC)150,150,115
115     IF(DX1)140,140,130
120     DFT=DFT/2.
125     IF(DX1)140,140,130
130     T4(I)=T4(I)-DFT
      GO TO 110
140     T4(I)=T4(I)+DFT
      GO TO 110
150     CONTINUE
      X1(I)= -(AKO+AK1/T1(I))*T4(I)**2.+AK2*(-T1(I)+1./T1(I))*T4(I)**3.
      I+T4(I)*T1(I)/(CZ*(1.-B1*T4(I)+B2*T4(I)*T4(I)))
160     TT=ALOG(TT=ALOG(T1(I)*TC/TO)
      TT1=1./((T1(I)*TC)-1./TO)
      TCP2=16.2*(T1(I)*TC-TO)-6530.*TT-1410000.*TT1
      X2(I)=-CZ*R*TC*T1(I)*(T4(I)*(2.*AKO/T1(I)+3.*AK1/T1(I)**2.))-
      1OZ*R*TC*T1(I)*(AK2*T4(I)*T4(I)*(1.-2./T1(I)**2.))+R*TC*T1(I)*B1*
      2T4(I)-B2*T4(I)*T4(I))/(1.-B1*T4(I)+B2*T4(I)*T4(I))+AH+TCP2
      X3(I)=1.2*X2(I)-0.2*X4(I-1)
      DX3=1.
170     CONTINUE
      DGT=0.002
      BX1=1.

```

```

175  XIC  =-(AXO+AK1/T2(I))*T5(I)**2.+AK2*(-T2(I)+1./T2(I))*T5(I)**3.
      1+T5(I)*T2(I)/(CZ*(1.-B1*T5(I)+B2*T5(I)*T5(I)))
      BX1P=BX1
      BX1=X1(1)-X1C
      IF(ABS (BX1)-AB1220,330,180
180  IF(BX1P*DX1) 185,185,190
185  DGT=DGT/2.
190  IF(BX1)200,200,210
200  T5(I)=T5(I)-DGT
      GO TO 175
210  T5(I)=T5(I)+DGT
      GO TO 175
220  CONTINUE
      TT=ALOG(T2(I)*TC/TO)
      TT1=1./T2(I)*TC)-1.TO
      TCP9=16.2*(T2(I)*TCOTI(06539,*TT01419999,*TT1
      X3C  --CZ*R*TC*T2(I)*(T5(I)*(2.*AKO/T2(I)+3.*AK1/T2(I)**2.))
      1CZ*R*TC*T2(I)*(AK2*T5(I)*T5(I)(1.-2./T2(I)**2.))+R*TC*T2(I)*(B1*
      2T5(I)-B2*T5(I)*T5(I))/(1.B1*T5(I)+B2*T5(I)*T5(I))+AH+TCP9
      DX3P=DX3
      DX3=X3(I)-X3C
      IF(ABS(DX3)-AD) 255,255,225
225  IF(DX3P*DX3) 230,230,235
230  DHT=DHT/2.
235  IF(DX3) 240,240,250
240  T2(I)=T2(I)-DHT
      GO TO 170
250  T2(I)=T2(I)+DHT
      GO TO 170
255  CONTINUE
      IF(I.EQ.4) GO TO 295
      DX1=1.
260  XIC  =-(AKO+AK1/T3(I))*T6(I)**2.+AK2*(-T3(I)+1./T3(I))*T6(I)**3.
      1+T6(I)*T3(I)/CZ*(1.-B1*T6(I)+B2*T6(I)*T6(I)))
      DX1P=DX1
      DX1=X1(I)-X1C
      IF(ABS (DX1)-AB) 290,290,265
265  IF(DX1P*DX1) 270,270,275
270  DIT=DIT/2.
275  IF(DX1)280,280,285
280  T6(I)=T6(I)-DIT
      GO TO 260
285  T6(I)=T6(I)+DIT
      GO TO 260
290  CONTINUE
      IF(T3(I)-TWT) 292,292,293
292  T3(I)=TXI+0.0001
293  TT=ALOG(T3(I)*TC?TO)
      TT1=1./((T3(I)*TC)-I./TO)
      TCP3=16.2*(T3(I)*TC-TO)-6530.*TT-1410000.*TT1
      X4(I)= -CZ*R*TC*T3(I)*(T6(I)*(2.*AKO/T3(I)+3.*AK1/T3(I)**2.))-
      1CZ*P*TC*T3(I)*(AK2*T6(I)*T6(I)*(1.-2./T3(I)**2.))+R*TC*T3(I)*(B1*
      216(I)-B2*16(1)*T6(I))/(1.-B1*T6(I)+B2*T6(I)*T6(I))+AH+TCP3

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TCS3=16.2*TT6530.*TT1-705000.*(1./(T3(I)*TC)**2.-1./TO**2.)
X6(I)=R*(CZ*(-AK1*T6(I)/T3(I)**2.+0.5*AK2*T6(I)*T6(I)*(1.+
11./T3(I)**2.))-ALOG(T6(I)*T3(I))+0.5*ALOG(1.-B1*T6(I)+
2B2*T6(I)*T6(I))-AK3*ATAN (AK3)-AK3*ATAN (AK4*T6(I)-AK3)+ALOG(CZ))+
3R*ALOG(POC)+AS+TCS3
295 DELT=((T2(I)-TWO)-(T3(I)-TWI))/ALOG((T2(I)-TWO)/(T3(I)-TWI))
X7(I)=X7(I-1)+CE*(X3(I)-X4(I-1))+PH*CHP*(X3(I)-X4(I-1))+PH*CH*
1(X3(I)-X4(I))/(O*C*DELT)+CH*(X3(I)-X4(I))/CPW*TC*(TWO-TWI))
WRITE(3,1002) 11(1),T2(I),T3(I),T4(I),T5(I),T6(I)
WRITE(3,1002) X1(1),X2(I),X3(I),X4(I),X5(I),X6(I),X7(I)
IF(I.EQ.4) GO TO 400
300 CONTINUE
T=4
GO TO 5
305 DFT=0.002
BX1=1.
310 X1C = -(AK0+AK1/T1(I))*T4(I)**2.+AK2*(-T1(I)+1./T1(I))*T4(I)**3.
1+T4(I)*T1(I)/(CZ*(1.-B1*T4(I)+B2*T4(I)*T4(I)))
BX1P=BX1
BX1=XI(I)=X1C
IF(ABS(BX1)-AB) 350,350,315
315 IF(BX1P*BX1) 320,320,325
320 DFT=DFT/2.
325 IF(BX1) 330,330,340
330 T4(I)=T4(I)-DFT
GO TO 310
340 T4(I)=T4(I)+DFT
GO TO 310
350 CONTINUE
TT1=1./(T1(I)*TC)-1./TO
TT=ALOG(T)(I)*TC/TO
TCP2=16.2*(T1(I)*TC-TO)-6530.*TT-1410000.*TT1
TCS2=16.2*TT+6530.*TT1-705000.*(1./(T1(I)*TC)**2.-1./TO**2.)
X5C = R*(CZ*(-AK1*T4(I)/T1(I)**2.+0.5*AK2*T4(I)*T4(I)*(1.+
11./T1(I)**2.))-ALOG(T4(I)*T1(I))+0.5*ALOG(1.-B1*T4(I)+
2B2*T4(I)*T4(I))-AK3*ATAN (AK3)-AK3*ATAN (AK4*T4(I)-AK3)+ALOG(CZ))+
3B*ALOG(POC)+AS+TCS2
DX5P=DX5
DX5=X5(I)-X5C
IF(ABS(DX5)-AC) 390,390,355
355 IF(DX5P*DX5) 360,360,365
360 DJT=DJT/2.
365 IF(DX5) 370,370,380
370 T1(I)=T1(I)-DJT
GO TO 305
380 (1)(I)=T1(I)+DJT
GO TO 305
390 CONTINUE
GO TO 160
400 DO 440 K=2,4
TP1=1.-B1*T4(K)+B2*T4(K)*T4(K)
TP2=T4(K)*T4(K)*T4(K)

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X1T1(K)=AK1*T4(K)*T4(K)/T1(K)**2-AK2*TP2-AK2*TP2/T1(K)**2
I+T4(K)/O/*TP1)
X1T4(K)=-2.*AKO+AK1/T1(K))*T4(K)+3.*AK2*(-T1(K)+1./T1(K))*
1T4(K)*T4(K)+(TP1*T1(K)-T4(K)*T1(K)*(-B1+2.*B2*T4(K)))/
2(OZ*TP1*TP1)
CP1=16.2- 6530./((TC*T10K))+ 1410000./((TC*T1(K))**2)
X2T1(K)=CZ*R*TC*3.*AK1*T(K)/(T1(K)*T1(K))-CZ*R*TC*AK2*T4(K)*
1T4(K)-2.*CZ*R*TC*AK2*T4(K)*T4(K)/(T1(K)*T1(K))+
2K*TC*(81*T4(K)-B2*T4(K))/4(K))/TP1 +CP1*TC
X2T4(K)=CZ*R*TC*T1(K)*12.*AKO/T1(K)+3.*AK1/(T1(K)*T1(K))-
12.*CZ*R*TC*T1(K)*AK2*T4(K)*(1.-2./(T1(K)*T1(K)))+
2K*TC*T1(K)*(B1-2.*B2*T4(K))/TP1*TP1)
410 TP3=1. -B1*T5(K)+B2*T5(K)*T5(K)
CP2=16.2- 6530./((TC*T2(K))+ 1410000./((TC*T2(K))**2)
X3T2(K)=CZ*R*TC*3.*AK1*T5(K)/(T2(K)*T2(K))-CZ*R*TC*AK2*T5(K)*T5(K)
1-2.*CZ*R*TC*AK2*T5(K)*T5(K)/T2(K)*T2(K))+R*TC*(81*T5(K)-
282*T5(K)*T5(K))/TP3 +CP2*TC
X3T5(K)=-CZ*R*TC*T2(K)*(2.*AKO/T2(K)+3.*AK1/(T2(K)*T2(K)))-
12.*CZ*R*TC*T2(K)*AK2*T5(K)*(1.-2./(T2(K)*T2(K)))+
2R*TC*T2(K)*(B1-2.*B2*T5(K))/TP3*TP3)
TP4=1.-B1*T6(K)+B2*T6(K)*T6(K)
CP3=16.2- 6530./((TC*T3(K))+ 1410000./((TC*T3(K))**2)
X4T3(K)=CZ*R*TC*3.*AK1*T6(K)/(T3(K)*T3(K))-CZ*R*TC*AK2*T6(K)*
1T6(K)-2.*CZ*R*TC*AK2*T6(K)*T6(K)/(T3(K)*T3(K))+R*TC*(B1*T6(K)-
2*2*T6(K)*T6(K))/TP4+CP3*TC
X4T6(K)=-CZ*R*TC*T3(K)*(2.*AKO/T3(K)+3.*AK1/(T3(K)*T3(K)))-
12.*CZ*R*TC*T3(K)*AK2*T6(K)*(1.-2./(T3(K)*T3(K)))+R*TC*T3(K)*
2(B1-2.*B2*T6(K))/TP4*TP4)
TP5=T1(K)*T1(K)*T1(K)
X5T1(K)=R*(CZ*(2.*AK1*T4(K)/TP5-AK2*T4(K)*T4(K)/TP5)-1./T1(K))+
1CP1/T1(K)
TP6=T3(K)*T3(K)*T3(K)
X6T3(K)=R*(C2*(2.*AK1*T6(K)/TP6-AK2*T6(K)*T6(K)/TP6)-1./T3(K))+
1CP3/T3(K)
420 X5T4(K)=R*(CZ*(-AK1/T1(K)**2.AK2*T4(K)*(1.+1.T1(K)**2.))-1./
1T4(K)-B1-2.*B2*T4(K))/(2.*(1.-B1*T4(K)+B2*T4(K)*T4(K)))-AK3*AK4.
2(1.+(AK4*T4(K)-AK3)*(AK4*T4(K)-AK3)))
X6T6(K)=R*(CZ*(-AK1/T3(K)**2.+AK2*T6(K)*(1.+1./T3(K)**2.))-1./
1T6(K)-(B1-2.*B2*T6(K))/(2.*(2.-B1*T6(K)+B2*T6(K)*T6(K)))-
2AK3*AK4/(1.+(AK4*T6(K)-AK3)*(AK4*T6(K)-AK3)))
XWRITE(3,1002) X1T1(K),X1T4(K),X2T1(K),X2T4(K)
X7T2(K)=X3T2(K)*CE+PH*CHP+CW/(CPW*TC*(TWO-TWI))+PH*CH*(
1ALOG(T2(K)-TWO)-ALOG(T3(K)-TWI))/(U*TC*((T2(K)-TWO)-(T3(K)-TWI)))
2+PH*CH*(X3(K)-X4(K))*((T2(K)-TWO)-(T3(K)-TWI)-(ALOG(T2(K)-TWO)-
3ALOG(T3(K)-TWI)))*(T2(K)-TWO))/O*TC*((T2(K)-TWO)-(T3(K)-TWI))*
4((I2(K)-TWO)-(T3(K)-TWI))*(T2(K)-TWO))
WRITE(3,1002) X3T2(K),X3T5(K)
X7T3(K)=X4T3(K)*(PH*CH*(ALOG(T2(K)-TWO)-ALOG(T3(K)-TWI)))/
1(C*TC*((T2(K)-TWO)-(T3(K)-TWI)))+CW/(CPW*TC*(TWO-TWI)))-
2PH*CH*(X3(K)-X4(K))*((T2(K)-TWO)-(T3(K)-TWI)+(T3(K)-TWI))*
3(ALOG(T2(K)-TWO)-ALOG(T3(K)-TWI)))/(O*TC*((T2(K)-TWO)-
4(T3(K)-TWI))*((T2(K)-TWO)-T3(K)-TWI))*(T3(K)-TWI))
XWRITE(3,1002) X4T3(K),X4T6(K),X5T1(K),X6T3(K)

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430 X7T5(K)=X3T5(K)*(CE+PH*CHP+CW/(CPW*TC*(TWO-TWI))+PH*CHP*
1 (ALOG(I2(K)-TWO)-ALOG(T3(K)-TWI))/(O*TC*((T2(K)-TWO)-(T3(K)-TWI)))
2)
WRITE(3,1002 X5T4(K),X6T6(K),X7I2(K),X7T3(K)
X7I6(K)=-X4I6(K)*(PH*CH*(ALOG(I2(K)-TWO)-ALOG(T3(K)-TWI)))/
1(O*TC*((T2(K)-TWO)-T3(K)-TWI))+CW/(CPW*TC*(TWO-TWI)))
X7X4(K)=- (CE+PH*CHP)
P1T1(K)=X1T1(K)
P1T2(K)= -(AK1*T5(K)**2)/(T2(K)**2) +AK2*(T3(K)**3)+AK2*(T5(K)**3)
1/(T2(K)**2)-T5(K)/(CZ*TP3)
P1T4(K)=X1T4(K)
P1T5(K)= 2.*(AKO+AK1/T2(K))*T5(K)-3.*AK2*(-T2(K)+1./T2(K))
1*T5(K)*T5(K)-(TP3*T2(K)-T5(K)*T2(K)*(-B1+2.*B2*T5(K)))
2/(CZ*TP3*TP3)
P2T4(K)=X1T4(K)
P2T1(K)=X1T1(K)
P2T6(K)= 2.*(AKO+AK1/T3(K))*T6(K)-3.*AK2*(-T3(K)+1./T3(K))
1/T3(K)**2-T6(K)/(CZ*(1.-B1*T6(K)+B2*T6(K)**2)___
P3T1(K)=X5T1(K)
P3T4(K)=X5T4(K)
P3X6(K)=-1.
P4T1(K)=-1.2*X2T1(K)
P4T2(K)=X3T2(K)
P4T4(K)=-1.2*(X2T4(K))
P4T5(K)=X3T5(K)
P4X4(K)=0.2
440 CONTINUE
Z2(4)=0.0
Z3(4)=0.0
Z4(4)=0.0
Z5(4)=0.0
Z6(4)=0.0
Z7(4)=1.0
ALM2(4)=-X7T6(4)/P2T6(4)/P2T6(4)
ALM4(4)=(X7T5(4)*P1T2(4)-X7T2(4)*P1T5(4))/(P4T2(4)*P1T5(4)-
1P4T5(4)*P1T2(4))
ALM1(4)=- (X7T2(4)+ALM4(4)*P4T1(4))/P1T2(4)
ALM3(4)=(X1T1(4)*(ALM1(4)*P1T4(4)+ALM3(4)*P2T4(4)+
1ALM4(4)*P4T4(4))-X1T4(4)*(ALM1(4)*P1T1(4)+ALM2(4)*P2T1(4)+
2ALM4(4)*P4T1(4)))/(P3T1(4)*X1T4(4)-P3T4(4)*X1T1(4))
Z1(4)=- (ALM1(4)*P1T1(4)+ALM2(4)*P2T1(4)+ALM3(4)*P3T1(4)+
1ALM4(4)*P4T1(4))/X1T1(4)
DO 490 K=2,3
I=5-K
Z1(I)=0.0
Z2(I)=0.0
Z3(I)=0.0
Z4(I)=- (CE+PH*CHP) +ALM4(I+1)*0.2
Z5(I)=0.0
Z6(I)=-ALM3(I+1)
Z7(I)=1.

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ALM3(1)=- (Z4(I)*X4T6(1)+Z6(I)*X6T6(I)+      X7T6(I))/P2T6(I)
ALM4(I)=(      X7T5(1)*P1I2(I)-      X7T2(I)*P1T5(I))/
1(P4T2(I)*P1I5(I)-P4T5(I)*P1T2(I))
ALM1(I)=- (ALM4(I)*P4T5(I)+      X7T5(I))/P1T5(I)
ALM3(I)=- (ALM1(I)*P1T4(I)+ALM2(I)*P2T4(I)+ALM4(I)*P4T4(I))/P3T4(I)
BI=HT1(I)
HT1(I)=ALM1(I)*P1T1(I)+ALM2(I)*P2T1(I)+ALM3(I)*P3T1(I)+
1ALM4(I)*P4T1(I)
WRITE(3,1002) T1(I),HT1(1)
DB=T1(1)-T1P(I)
T1P(1)=T1(I)
IF(ABS(DD)-0.002) 450,450,443
448 IF(HT1(I)*H1 ) 445,445,450
445 DK(I)=DKT(I)/2.
450 IF(HT1(I)) 455,455,460
455 T1(I)=T1(I)+DKT(I)
GO TO 465
460 T1(I)=T1(I)-DKT(I)
465 H3 =HT3(I)
HT3(I)=Z4(I)*X4T3(I)+Z6(I)*X6T3(I)+ X7T3(I)+ALM2(I)*P2T3(I)
WRITE(3,1002) T3(I),HT3(I)
DO=T3(I)=T3(I)
IF(ABS(DD)-0.002) 475,475,468
468 IF(HT3(I)*H3 ) 470,470,475
470 DLT(I)=DLT(I)/2.
475 IF(HT3(I)) 480,480,485
480 T3(I)=T3(I)+DLT(I)
GO TO 490
485 T3(I)=T3(I)-DLT(I)
490 CONTINUE
WRITE(3,1002)(Z1(I),Z2(I),Z3(I),Z4(I),Z5(I),Z6(I),Z7(I),I=2,4)
WRITE(3,1002)(ALM1(I),ALM2(I),ALM3(I),ALM4(I),I=2,4)
WRITE(3,1002)HT1(2),HT3(2)
WRITE(3,1002),HT1(3),HT3(3)
GO TO 4
500 CONTINUE
GO TO 2
510 CONTINUE
GO TO 1
520 STOP
END

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CHAPTER 7. RECOMMENDATION FOR FUTURE WORK

The system analysis and the computational algorithm developed in this study are fairly general and are adaptive to changes in the equation of state, and changes in the cost models. Therefore, the present approach can be applied to any gas and can be extended to any gas mixture and to any operating range by proper selection of the equation of state. In the cost analysis of this work, linear cost relations have been used for the compressors and the intercoolers. These assumptions have been introduced not because of the limitation of the methods, but because of the lack of cost information required to establish better cost models.

The following studies are recommended for future work.

1. Establishment of realistic cost model. The manufacturers should be contacted to establish the cost models for the compressors and the intercoolers. The cost model for compressors should show the variations in the compressor cost with respect to the changes in the operating pressure and the capacity. The intercooler cost should also vary with the operating pressure and vary non-linearly with the heat transfer area.
2. Extension of the operating range. In this study, numerical calculations have been carried out for CO₂ gas compression within range I (low density gas). The computations can be extended to gas compressions spanning among two or more ranges.

3. Use of other equations of state. The approach used in this study is quite general. Therefore, any equation of state may be used to establish the performance equations.
4. Improvement of root finding methods. It has been shown that quite often we have to find roots for implicit functions in using the present method. Other root finding methods or search techniques may be more efficient than the interval halving method which has been used here.

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SYSTEM ANALYSIS AND OPTIMIZATION STUDY OF
A MULTISTAGE GAS COMPRESSION SYSTEM

by

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The primary objective of this study is to improve the system analysis and optimization study of a multistage gas compression system. In this study, we take into consideration the non-ideal behavior of a gas and irreversibilities of the compressors. Furthermore, we include the first costs of the interstage coolers and pumps, the cooling water cost and energy cost in the objective function. The optimization technique developed in this study is based on the discrete analog of the maximum principle and an iterative search method. The technique employs four Lagrange multipliers in each stage in association with four constraint relations. The method developed is quite general and can be used in combination with any equation of state.

The equation of state developed by J. O. Hirshfelder et al. is used and numerical computation is illustrated by 3-stage gas compression of carbon dioxide. The numerical computations have shown the following significant results:

1. The optimal policy of a multistage gas compression system is affected not only by the discharge pressure but also by the discharge temperature.
2. The optimal policy of a three stage carbon dioxide gas compression system as computed by the present approach is significantly different from the policy as computed by the conventional approaches.
3. The gas compression cost evaluated at the optimum condition as determined by the present approach is significantly lower than the gas compression cost evaluated at the optimum condition as determined by the conventional approaches. The difference in these

costs increases as the discharge pressure increases. The cost saving is about 2.5% for CO₂ compression at discharge pressure of 1700 psi.

All the numerical computation has been made by IBM 360 computer, and one iteration takes 20 seconds of computer time. Assuming that 15 iterations are required to arrive at the optimum policy, the computer time required is 5 minutes for solving an optimization problem.

