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Optimum Thrust Nozzle Contours For Chemically Reacting Gas Flows

by

Joe D. Hoffman

Technical Memorandum
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JET PROPULSION CENTER
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ABSTRACT

An optimization analysis is presented for the design of axisymmetric rocket motor nozzles with chemically reacting gas flows. The analysis is based upon the usual assumptionsfor reacting flows. An arbitrary number of chemical species and chemical reactions are included in the analysis. The problem is formulated to maximize the pressure thrust integral along the supersonic nozzle wall contour for a general isoperimetric constraint, such as constant nozzle length or constant nozzle surface area. The governing partial differential equations for reacting flows are incorporated into the analysis by means of Lagrange multipliers. The results of the optimization analysis are a set of partial differential equations for determining the Lagrange multipliers in the region of interest, and a set of algebraic equations for determining initial conditions for these Lagrange multipliers on the boundaries of the region. It is shown that the complete set of equations for the gasdynamic properties and the Lagrange multipliers constitutes a system of first order, quasi-linear, non-homogeneous partial differential equations of the hyperbolic type, which can be treated by the method of characteristics. The characteristic and compatibility equations for the system are presented. A technique for employing the results to determine optimum thrust nozzle contours is presented.

I. INTRODUCTION

Many high energy propellant combinations used in propulsion engines experience a considerable difference between the predicted performance based upon isentropic shifting equilibrium and the actual performance. These losses are due both to the presence of boundary layers and to the nonequilibrium processes associated with chemical recombination lags, thermodynamic relaxation, and velocity and thermal lags associated with the flow of condensed phases. In the process of supersonic combustion, the losses associated with the nonequilibrium process of chemical relaxation can completely determine the success or failure of the system. In view of the important effect of the chemical recombination process in the exhaust nozzle of both rocket engines and air breathing engines, it is obvious that the nozzle design must be given careful consideration.

The Jet Propulsion Center, Purdue University, has had a continuing interest in both nozzle analysis and design techniques for several years, as evidenced by references 1 through 13. A recent paper by Thompson and Murthy[8] presents an optimization technique for the design of three-dimensional nozzles for homentropic, perfect gas flows. The present analysis presents an optimization technique for the design of axisymmetric nozzles whose working fluid is a chemically reacting gas.

The first attempt at nozzle design by applying optimization techniques was made by Guderley and Hantsch[14] for an axisymmetric, hometropic flow in a nozzle of fixed length. Rao[15] later considered the same problem as that investigated by Guderley and Hantsch, and developed a design technique which has proven to be much easier to apply. As a result, Rao's technique is in wide use throughout the rocket industry. Guderley[16] analyzed the differences between the approaches of references 14 and 15, and extended the analysis to axisymmetric, isentropic flows with non-constant entropy between streamlines. All of these analyses were based on a one-dimensional control surface, illustrated in Fig. 1, consisting of the left running Mach line BC which passes through the nozzle exit. This approach is permissible when no dissapative effects are present in the flow field, so that all the thermodynamic properties along the control surface can be determined uniquely as a function of the velocity of the flow. Effectively, the path taken by a streamline does not affect the relationship between thermodynamic variables and flow velocity.

Guderley and Armitage[17,18] formulated the problem of obtaining the optimum contour for a fixed nozzle surface area. In this approach, the entire region ABC in Fig. 1 must be considered. Although this analysis was also restricted to a non-dissapative flow field, the technique can be employed for dissaptive flows since the entire flow field is included in the optimization analysis. The present analysis is based upon the techniques developed in references 17 and 18.

Appleton[19] presented a one-dimensional relaxation technique for minimizing the recombination losses in a nozzle. No account is taken of the two-dimensional effects in the nozzle or the exit divergence loss. Burwell et al.[20] developed a design technique based upon a two-dimensional analysis of a reacting flow in truncated perfect nozzles. This technique

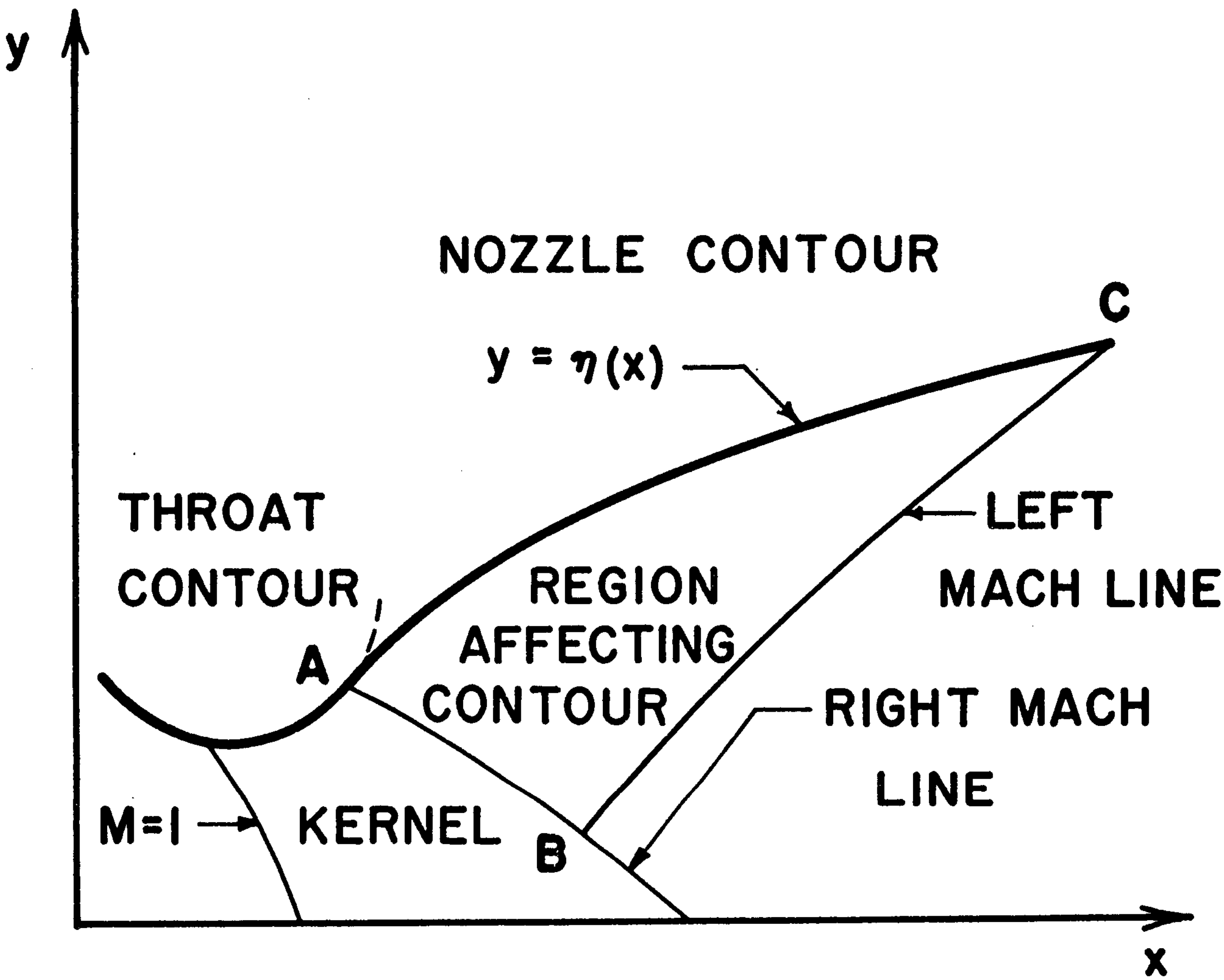

FIGURE 1. MODEL FOR OPTIMIZATION TECHNIQUES

has no guarantee of producing the optimum contour, although the results obtained by such an approach are very useful. The present analysis is an improvement in that the two-dimensional nature of the flow is accounted for, and the optimum contour is obtained by employing the techniques of the calculus of variations.

II. TECHNICAL DEVELOPMENT

A. Analysis of Chemically Reacting Flows

The present analysis is based upon the usual assumptions for axisymmetric chemically reacting flows as discussed in references 21, 22, and 23. The optimization procedure will be applied only to the supersonic portion of the nozzle. Hence, the flow field up to the supersonic region must be known. As discussed by Der[22] and Craig,[23] the flow in the subsonic portion of the nozzle can be treated by one-dimensional techniques to determine a transonic initial value line. The method of characteristics can then be employed to obtain the flow field downstream of the throat, thus establishing a known flow field with which the optimization procedure can be initiated.

The equations governing the axisymmetric flow of a chemically reacting gas are developed in Appendix A in a form suitable for the present application. This set of equations is valid for any number of chemical species and any number of chemical reactions. The following system of equations is applicable.

$$\rho u_x + \rho v_y + u\rho_x + v\rho_y = -\frac{\rho v}{y} \tag{1}$$

$$\rho u u_x + \rho v u_y + P_x = 0 \tag{2}$$

$$\rho u v_x + \rho v v_y + P_y = 0 \tag{3}$$

$$uP_x + vP_y - a^2u\rho_x - a^2v\rho_y = \sum_{i=1}^{n} \psi_i(P,\rho,C_k) \tag{4}$$

$$\rho u(C_i)_x + \rho v(C_i)_y = \sigma_i(P,\rho,C_k) \qquad (i = 1,..,n) \tag{5}$$

$$\sigma_i = W_i \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left[K_{fr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu'_{jr}} - K_{rr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu''_{jr}} \right] \tag{6}$$

$$\sum_{i=1}^{n} \psi_i = \sum_{i=1}^{n} \left[\gamma R_i T - (\gamma-1)h_i\right] \sigma_i \tag{7}$$

$$P = \rho T \sum_{i=1}^{n} C_i R_i \tag{8}$$

$$h = \sum_{i=1}^{n} C_i h_i \tag{9}$$

$$h_i = \int_{T_o}^{T} C_{pi} dT + h_i^o \tag{10}$$

The species source function σ_i was obtained from the law of mass action. The forward and reverse reaction rate constants, K_{fr} and K_{rr}, are obviously functions of temperature. However, variations in temperature can be expressed as variations in P, ρ, and C_k by employing the perfect gas law, Eq. (8). In the present analysis, this substitution has been made so that variations in σ_i can be expressed in terms of variations in P, ρ, and C_k. Similar comments apply to the function ψ_i, defined by Eq. (7). In the terms $\sum \psi_i(P,\rho,C_k)$ and $\sigma_i(P,\rho,C_k)$, the term C_k denotes that the function involved depends upon all n of the mass fractions.

The flow of a chemically reacting gas is completely described by the above set of equations, Eqs. (1) through (10). These equations will be incorporated into the optimization analysis to insure that a physically realizable solution is obtained.

B. Formulation of the Optimization Problem

In the present analysis of optimum thrust nozzle contours for chemically reacting gas flows, only the supersonic portion of the nozzle can be optimized. The subsonic and transonic nozzle contours must be prescribed beforehand, and the optimum nozzle contour obtained is then the best contour for that particular choice of subsonic and transonic geometrics only. This restriction has been employed by Guderley[14,16,17,18] and Rao[15] in their nozzle optimization studies involving inert gas flows.

The model to be considered as illustrated in Fig. 1. The right running characteristic AB originating at point A on the nozzle wall separates the flow field into the upstream region which is fixed by the given subsonic and transonic contours, and the downstream region which will be affected by variations in the nozzle contour. The nozzle ends at point C, and the left running Mach line BC passing through point C intersects the right running Mach line AB at point B.

The thrust developed by the portion of the nozzle between A and C is determined by integrating the pressure forces acting on the nozzle wall AC. The flow field beyond the left running Mach line BC will have no effect on the nozzle thrust, and need not be considered in the analysis. The problem then becomes the determination of the optimized nozzle contour, $y = \eta(x)$, which develops maximum thrust for the given subsonic and transonic contours subject to some restrictions on the allowable supersonic contour, for example, fixed nozzle length, fixed nozzle surface area, etc. The optimum nozzle contour is obtained by applying the techniques of the calculus of variations to the flow field in region ABC.

The thrust term to be maximized along AC is given by

$$F = \frac{\text{Thrust}}{2\pi} = \int_A^C (P-P_o)\ \eta\eta'\ dx \tag{11}$$

where $y = \eta(x)$ is the desired optimum contour. The engineering aspect of the problem enters through the specification of a general isoperimetric constraint $G(\eta,\eta',P)$ which is imposed on the nozzle contour by forcing the integral of $G(\eta,\eta',P)$ along AC to be constant. The general isoperimetric constraint is specified by the following equation.

$$S = \int_A^C G(\eta,\eta',P)\ dx = \text{Constant} \tag{12}$$

The function G can be specified at the discretion of the nozzle designer. Examples of constant length, constant arc length, constant surface area, and constant weight are presented in Section II. E. The line AC along which the thrust is to be maximized is forced to be a gas streamline by including the equation of a streamline, multiplied by $\eta\rho$ to simplify future manipulations, as a constraint.

$$\eta\rho(u\eta' - v) = 0 \qquad \text{on AC} \tag{13}$$

In order to insure that the solution obtained is physically possible, the equations which govern the flow of a chemically reacting gas are introduced into the optimization problem as constraints by means of Lagrange multipliers. Equations (1) through (4) can be represented symbolically by the differential operator L_j.

$$L_j(x,\ y,\ u,\ v,\ P,\ \rho,\ C_k) = 0 \qquad\qquad (j = 1,\ldots,4) \qquad\qquad (14)$$

Equation (5) can be represented symbolically by the differential operator M_i.

$$M_i(x,\ y,\ u,\ v,\ P,\ \rho,\ C_k) = 0 \qquad\qquad (i = 1,\ldots,n) \qquad\qquad (15)$$

The thrust is to be maximized by allowing arbitrary variations in the following parameters.

$$\begin{array}{lllll} u(x,y) & P(x,y) & \eta(x) & C_i(x,y) & (i = 1,\ldots,n) \\ v(x,y) & \rho(x,y) & X_c & & \end{array} \qquad (16)$$

The ext~~ernal~~remal problem is formulated in terms of the following expression, which is to be held stationary.

$$F + C_1S + \int_A^C C_2(x)\eta\rho(u\eta' - v)\ dx + \iint_{ABC} \sum_{j=1}^{4} h_j(x,y)\ L_j\ dxdy + \\ + \iint_{ABC} \sum_{i=1}^{n} g_i(x,y)\ M_i\ dxdy \qquad (17)$$

where C_1, C_2, h_j, and g_i are Lagrange multipliers. The above expression is required to be stationary for arbitrary variations in the parameters listed in Eq. (16). When expanded, Eq. (17) has the following form.

$$\int_A^C \{ (P-P_o)\eta\eta' + C_1 G(\eta,\eta',P) + C_2(x)\eta\rho(u\eta'-v) \} dx +$$

$$+ \iint_{ABC} \Big\{ h_1(x,y) \; [(y\rho u)_x + (y\rho v)_y] +$$

$$+ h_2(x,y) \; [\rho u u_x + \rho v u_y + P_x] + h_3(x,y) \; [\rho u v_x + \rho v v_y + P_y] +$$

$$+ h_4(x,y) \; [uP_x + vP_y - a^2 u\rho_x - a^2 v\rho_y - \sum_{i=1}^{n} \psi_i(P,\rho,C_k)] +$$

$$+ \sum_{i=1}^{n} g_i(x,y) \; [\rho u(C_i)_x + \rho v(C_i)_y - \sigma_i(P,\rho,C_k)] \Big\} dxdy \quad (18)$$

In order to reduce the algebraic complexity of the analysis, variations will not be taken in all of the parameters simultaneously. Variations in u, v, P, ρ, and C_k are taken in Section II.C., and variations in the nozzle contour $\eta(x)$ and end point X_c are taken in Section II.D. This procedure is permissible since all the variations are independent of each other. The results obtained after taking all of the variations are summarized in Section II.F.

C. Variations of Gas Properties

A detailed development of the results presented in this section is presented in Appendix B. Taking variations of u, v, P, ρ, and C_k in Eq. (18) results in the following expression.

$$\int_A^C \{\eta\eta'\delta P + C_1 G_p \delta P + C_2 \eta\rho(\eta'\delta u - \delta v)\}\, dx +$$

$$+ \iint_{ABC} \Bigg\{ h_1 \left[\frac{\partial}{\partial x}\,\delta(y\rho u) + \frac{\partial}{\partial y}\,\delta(y\rho v) \right] +$$

$$+ h_2 \left[\delta(\rho u u_x) + \delta(\rho v u_y) + \frac{\partial}{\partial x}\,\delta P \right] +$$

$$+ h_3 \left[\delta(\rho u v_x) + \delta(\rho v v_y) + \frac{\partial}{\partial y}\,\delta P \right] +$$

$$+ h_4 \Bigg[\delta(uP_x) + \delta(\overset{v}{\cancel{\rho}}P_y) - \delta(a^2 u\rho_x) - \delta(a^2 v\rho_y) -$$

$$- \sum_{i=1}^{n} \psi_{iP}\delta P - \sum_{i=1}^{n} \psi_{i\rho}\delta\rho - \sum_{i=1}^{n} \left\{ \sum_{k=1}^{n} (\psi_k)_{C_i} \right\} \delta C_i \Bigg] +$$

$$+ \sum_{i=1}^{n} g_i \left[\delta\{\rho u(C_i)_x\} + \delta\{\rho v(C_i)_y\} \right] - \sum_{i=1}^{n} g_i \left\{ \sum_{k=1}^{n} (\sigma_i)_{C_k} \delta C_k \right\} -$$

$$- \sum_{i=1}^{n} g_i \sigma_{iP}\delta P - \sum_{i=1}^{n} g_i \sigma_{i\rho}\delta\rho \Bigg\}\, dxdy = 0 \tag{19}$$

The following expansion of the terms in the second line of Eq. (19) is applicable in region ABC.

$$\delta(y\rho u) = y\rho\delta u + yu\delta\rho \tag{20}$$

$$\delta(y\rho v) = y\rho\delta v + yv\delta\rho \tag{21}$$

The frozen speed of sound appearing in Eq. (19) is given by

$$a^2 = \gamma RT = C_p RT/C_v = \frac{C_p P}{C_v \rho} \tag{22}$$

Taking variations of Eq. (22) yields

$$\delta a^2 = a^2 \sum_{i=1}^{n} a_i \delta C_i + \frac{a^2}{P} \delta P - \frac{a^2}{\rho} \delta \rho \tag{23}$$

where

$$a_i = \frac{1}{C_P} (C_{Pi} - \gamma C_{vi}) \tag{24}$$

Substituting Eqs. (20), (21) and (23) into Eq. (19), and applying Green's theorem in the plane to the terms under the integral over region ABC, the following result is obtained.

$$\left(\begin{aligned} & \int_A^C \left\{ \eta\eta' \delta P + C_1 G_P \delta P + C_2 \eta\rho (\eta' \delta u - \delta v) \right\} dx + \\ & + \left\{ \int_A^C - \int_B^C - \int_A^B \right\} \Big\{ h_1 y\rho\delta v + h_1 y v \delta\rho + h_2 \rho v \delta u + h_3 \rho v \delta v + \\ & \qquad + h_3 \delta P + h_4 v \delta P - h_4 a^2 v \delta\rho + \rho v \sum_{i=1}^{n} g_i \delta C_i \Big\} dx - \\ & - \left\{ \int_A^C - \int_B^C - \int_A^B \right\} \Big\{ h_1 y \rho \delta u + h_1 y u \delta\rho + h_2 \rho u \delta u + h_3 \rho u \delta v + \\ & \qquad + h_2 \delta P + h_4 u \delta P - h_4 a^2 u \delta\rho + \rho u \sum_{i=1}^{n} g_i \delta C_i \Big\} dy + \\ & + \iint_{ABC} \Big\{ \Big[-y\rho (h_1)_x + h_2 \rho u_x - (h_2 \rho u)_x - (h_2 \rho v)_y + h_3 \rho v_x + \\ & \qquad + h_4 P_x - h_4 a^2 \rho_x + \rho \sum_{i=1}^{n} g_i (C_i)_x \Big] \delta u + \\ & \quad + \Big[-y\rho (h_1)_y + h_2 \rho u_y + h_3 \rho v_y - (h_3 \rho u)_x - (h_3 \rho v)_y + \end{aligned} \right. \tag{25}$$

$$
\begin{aligned}
&+ h_4 P_y - h_4 a^2 \rho_y + \rho \sum_{i=1}^{n} g_i (C_i)_y \Big] \delta v + \\
&+ \Big[- h_4 \frac{a^2}{P} (u\rho_x + v\rho_y) - (h_2)_x - (h_3)_y - (h_4 u)_x - (h_4 v)_y - \\
&\quad - h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i \sigma_{iP} \Big] \delta P + \\
&+ \Big[-yu(h_1)_x - yv(h_1)_y + h_2 u u_x + h_2 v u_y + h_3 u v_x + h_3 v v_y + \\
&\quad + a^2 (h_4 u)_x + a^2 (h_4 v)_y + h_4 u a^2 \left\{ \sum_{i=1}^{n} a_i (C_i)_x + \frac{1}{P} P_x - \frac{1}{\rho} \rho_x \right\} + \\
&+ h_4 v a^2 \left\{ \sum_{i=1}^{n} a_i (C_i)_y + \frac{1}{P} P_y - \frac{1}{\rho} \rho_y \right\} + u \sum_{i=1}^{n} g_i (C_i)_x + \\
&\quad + v \sum_{i=1}^{n} g_i (C_i)_y - h_4 \sum_{i=1}^{n} \psi_{i\rho} - \sum_{i=1}^{n} g_i \sigma_{i\rho} \Big] \delta\rho + \\
&+ \sum_{i=1}^{n} \Big[-h_4 a^2 a_i (u\rho_x + v\rho_y) - (g_i \rho u)_x - (g_i \rho v)_y - \\
&\quad - h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} - \sum_{k=1}^{n} g_k (\sigma_k)_{C_i} \Big] \delta C_i \Big\} \, dxdy = 0
\end{aligned}
\qquad (25)
$$

Consider the line integrals appearing in Eq. (25). Note that along AC, where $y = \eta(x)$,

$$
\int_A^C f(y)\,dy = \int_A^C f\,[\eta(x)]\,\eta'\,dx \qquad (26)
$$

Substituting Eq. (26) into Eq. (25), and noting that the line integrals must equal zero independently of the surface integrals for arbitrary variations in the gas properties, the following equations are obtained.

$$\int_A^C \Big\{ [C_2\eta\rho\eta' + h_2\rho v - h_2\rho u\eta' - h_1\eta\rho\eta'] \, \delta u +$$

$$+ [-C_2\eta\rho + h_3\rho v + h_1\eta\rho - h_3\rho u\eta'] \, \delta v +$$

$$+ [\eta\eta' + h_3 + h_4 v - h_2\eta' - h_4 u\eta' + C_1 G_p] \, \delta P +$$

$$+ [-h_4 a^2 v + h_1\eta v + h_4 a^2 u\eta' - h_1\eta u\eta'] \, \delta\rho$$

$$+ \sum_{i=1}^{n} [\rho v g_i - \rho u\eta' g_i] \, \delta C_i \Big\} \, dx = 0 \qquad (27)$$

$$\Big\{\int_B^C + \int_A^B\Big\} \Big\{ [h_2\rho v dx - h_2\rho u dy - h_1 y\rho dy] \, \delta u +$$

$$+ [h_3\rho v dx - h_3\rho u dy + h_1 y\rho dx] \, \delta v +$$

$$+ [h_3 dx - h_2 dy + h_4 v dx - h_4 u dy] \, \delta P +$$

$$+ [-h_4 a^2 v dx + h_1 y v dx + h_4 a^2 u dy - h_1 y u dy] \, \delta\rho +$$

$$+ \sum_{i=1}^{n} [\rho v g_i dx - \rho u g_i dy] \, \delta C_i \Big\} = 0 \qquad (28)$$

Since the line integral in Eq. (27) must equal zero for arbitrary values of δu, δv, δP, $\delta\rho$, and δC_i, the coefficients of these variations must equal zero identically, resulting in the following relationships which are valid along the nozzle wall AC.

$$h_1 = C_2 \tag{29}$$

$$uh_3 - vh_2 + v\eta + uG_pC_1 = 0 \tag{30}$$

Since no variations in gas properties are allowed in the kernel, the variations in gas properties along right running characteristic AB will automatically be zero. Thus, the line integral along AB will be zero and no new conditions result along that line. However, the variations along the exit control characteristic BC are arbitrary. This requires that the coefficients of the variations in Eq. (28) be equal to zero, resulting in the following relationships which apply along the exit control characteristic BC.

$$yy'h_1 + (uy' - v)h_2 = 0 \tag{31}$$

$$yh_1 - (uy' - v)h_3 = 0 \tag{32}$$

$$yh_1 - a^2h_4 = 0 \tag{33}$$

$$g_i = 0 \qquad (i = 1, \ldots, \eta) \tag{34}$$

Returning to the surface integral appearing in Eq. (25), the variations in gas properties must be arbitrary over the region of integration. Hence, the coefficients of the variations must be identically zero. After some manipulation, including the substitution of the original system equations, Eqs. (1) through (4), the following set of partial differential equations for determining the Lagrange multipliers in region ABC is obtained.

$$-h_2u_x - h_3v_x - \frac{1}{\rho} h_4 (P_x - a^2\rho_x) + y(h_1)_x + u(h_2)_x + \\ + v(h_2)_y - \sum_{i=1}^{\eta} g_i(C_i)_x = K_1 \tag{35}$$

$$-h_2u_y - h_3v_y - \frac{1}{\rho} h_4 (P_y - a^2\rho_y) + y(h_1)_y + u(h_3)_x + \\ + v(h_3)_y - \sum_{i=1}^{\eta} g_i(C_i)_y = K_2 \tag{36}$$

$$h_4u_x + h_4v_y + h_4 \frac{a^2}{P} (u\rho_x + v\rho_y) + (h_2)_x + (h_3)_y + \\ + u(h_4)_x + v(h_4)_y = K_3 \tag{37}$$

$$\frac{1}{\rho} h_4 P_x + \frac{1}{\rho} h_4 P_y + yu(h_1)_x + yv(h_1)_y + a^2(h_2)_x + a^2(h_3)_x = K_4 \tag{38}$$

$$h_4a^2a_i(u\rho_x + v\rho_y) + \rho u(g_i)_x + \rho v(g_i)_y = J_i \qquad (i = 1, .., \eta) \tag{39}$$

$$K_1 = h_2 \frac{v}{y} \tag{40}$$

$$K_2 = h_3 \frac{v}{y} \tag{41}$$

$$K_3 = -h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i \sigma_{iP} \tag{42}$$

$$K_4 = h_4 \frac{a^2}{P} \sum_{i=1}^{n} \psi_i - h_4 \sum_{i=1}^{n} (a^2 \psi_{iP} + \psi_{i\rho}) - \sum_{i=1}^{n} g_i (a^2 \sigma_{iP} + \sigma_{i\rho}) +$$

$$+ \frac{1}{\rho} \sum_{i=1}^{n} (h_4 a^2 a_i + g_i)\, \sigma_i \tag{43}$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} - \sum_{k=1}^{n} g_k (\sigma_k)_{C_i} \qquad (i = 1,.., n) \tag{44}$$

Equations (1) through (5), together with Eqs. (35) through (39), constitute a system of (8+2n) partial differential equations for determining the (8+2n) variables u, v, P, ρ, C_i, h_1, h_2, h_3, h_4 and g_i. As shown in Appendix E, these (8+2n) equations form a system of quasi-linear, nonhomogeneous, first order partial differential equations of the hyperbolic type. Thus, this system of equations can be replaced by an equivalent system of characteristic and compatibility equations, which are total differential equations of the first order. The following characteristic system was obtained. Along gas streamlines,

$$\frac{dy}{dx} = \frac{v}{u} \tag{45}$$

$$\rho u du + \rho v dv + dP = 0 \tag{46}$$

$$dP - a^2 d\rho = \frac{1}{u} \sum_{i=1}^{n} \psi_i \; dx \tag{47}$$

$$\rho u dC_i = \sigma_i dx \qquad (i = 1,.., n) \tag{48}$$

$$-h_2du - h_3dv + ydh_1 + udh_2 + vdh_3 =$$

$$= K_1dx + K_2dy + \frac{1}{\rho u} h_4 \sum_{i=1}^{n} \psi_i dx + \frac{1}{\rho u} \sum_{i=1}^{n} g_i \sigma_i \, dx \qquad (49)$$

$$(vh_2 - uh_3)dv + \frac{1}{\rho} h_2 \, dP - h_4 \frac{a^2 u}{\rho} (\gamma - 1) \, d\rho + yudh_1 - ua^2 dh_4 =$$

$$= [-h_4 a^2 \frac{v}{y} - a^2 K_3 + K_4] \, dx \qquad (50)$$

$$udg_i = J_i dx - h_4 a^2 u a_i d\rho \qquad (i = 1, .., n) \qquad (51)$$

Along gas Mach lines,

$$\frac{dy}{dx} = \tan (\theta \pm \alpha) \qquad (52)$$

$$a^2 (vdu - udv) \pm \frac{1}{\rho} a^2 \cot\alpha \, dP = (udy - vdx) \left[a^2 \frac{v}{y} + \frac{1}{\rho} \sum_{i=1}^{n} \psi_i \right] \qquad (53)$$

$$h_2du + h_3dv + \frac{1}{\rho} h_4 (dP - a^2 d\rho) + \sum_{i=1}^{n} g_i dC_i - ydh_1 \mp$$

$$\mp \tan\alpha \, (vdh_2 - udh_3) = \pm \tan\alpha \, (K_2dx - K_1dy) \pm$$

$$\pm \frac{1}{a^2} \tan\alpha \, (udy - vdx) \left[K_4 + \frac{1}{\rho} h_4 \sum_{i=1}^{n} \psi_i \right] \qquad (54)$$

where θ is the flow angle and α is the Mach angle. In Eqs. (52), (53), and (54), the upper signs refer to left running Mach lines and the lower signs to right running Mach lines.

The terms K_3, K_4 and J_i defined in Eqs. (42), (43) and (44) involve complicated derivatives of the functions ψ_i and σ_i. After some lengthy manipulation, these terms can be expressed in terms of the fundamental thermodynamic properties of the system in the following form (See Appendix F).

$$K_3 = -h_4 \frac{C_p T}{P} \sum_{i=1}^{n} a_i \sigma_i - \frac{T}{P} \sum_{i=1}^{n} (h_4 \phi_i + g_i) W_i \times$$
$$\times \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left[\frac{dK_{fr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - \frac{dK_{rr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right] \quad (55)$$

$$K_4 = \frac{1}{\rho} \sum_{i=1}^{n} g_i \sigma_i + h_4 \frac{a^2}{P} \sum_{i=1}^{n} \psi_i - \frac{1}{\rho} \sum_{i=1}^{n} (h_4 \phi_i + g_i) W_i \times$$
$$\times \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left\{ \left[K_{fr} \sum_{j=1}^{n} \nu'_{jr} + (\gamma-1)\, T \frac{dK_{fr}}{dT} \right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - \right.$$
$$\left. - \left[K_{rr} \sum_{j=1}^{n} \nu''_{jr} + (\gamma-1)\, T \frac{dK_{rr}}{dT} \right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right\} \quad (56)$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} \left[\gamma (R_k T - h_k) a_i + \frac{C_p R_i T}{R} a_k \right] \sigma_k -$$
$$- \sum_{k=1}^{n} (h_4 \phi_k + g_k) W_k \sum_{r=1}^{N} (\nu''_{kr} - \nu'_{kr}) \left\{ \left[\frac{1}{C_i} K_{fr} \nu'_{ir} - \frac{R_i T}{R} \frac{dK_{fr}}{dT} \right] \times \right.$$
$$\left. \times \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - \left[\frac{1}{C_i} K_{rr} \nu''_{ir} - \frac{R_i T}{R} \frac{dK_{rr}}{dT} \right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right\}$$

$$(i = 1, \ldots, n) \quad (57)$$

In summary, the characteristic system defined by Eqs. (45) through (57) can be employed to evaluate the gasdynamic properties and the Lagrange multipliers throughout region ABC.

D. Variation in Nozzle Contour and End Point

Variations of the nozzle contour $\eta(x)$ and end point X_c are discussed in detail in Appendix ~~B~~ C. The limits of integration of the double integrals over region ABC in Eq. (18) are functions of the boundaries of these regions. Hence, arbitrary variations in these limits must be allowed. However, the integrands of these integrals are identically zero over the entire region of interest, including the boundaries of the region. Thus, the variations arising from the limits of integration of the double integrals can be arbitrary without introducing any new conditions into the problem.

The contour $\eta(x)$ and end point X_c also appear in the line integral along the nozzle wall AC in Eq. (18). The contour η enters both directly as a factor and also as the argument of all gas properties. For example,

$$u(x,y) = u[x,\eta(x)] \qquad \text{on AC} \tag{58}$$

Variations can be taken in all gas properties due to variations in η at fixed x. These variations are independent of those taken in the previous section which were taken at fixed x and y. Thus

$$\delta u = \frac{\partial}{\partial \eta}\left\{ u[x,\eta(x)] \right\} \delta\eta = u_y \delta\eta \tag{59}$$

Since the nozzle end point X_c appears in the limits of integration in Eq. (18), a variation in X_c must also be taken. Taking the variation in the limit of integration at point C in Eq. (18), and allowing δX_c to be arbitrary, gives

$$C_1 = -\frac{\eta_c\,\eta_c'\,(P_c - P_o)}{G(\eta_c,\,\eta_c',\,P_c)} \tag{60}$$

Taking the variation of η in the line integral in Eq. (18) yields the following result.

$$\int_A^C \left\{ \left[\eta\eta' P_y + (P-P_o)\eta' + C_1 G_\eta + C_1 G_P P_y + C_2\{\eta'(\eta\rho u)_y - (\eta\rho v)_y\} \right] \delta\eta + \right.$$
$$\left. + \left[(P-P_o)\eta + C_1 G_{\eta'} + C_2(\eta\rho u) \right] \delta\eta' \right\} dx = 0 \tag{61}$$

Substituting the continuity equation, Eq. (1), into Eq. (61), and integrating by parts the coefficient of $\delta\eta'$, gives the following equation.

$$\left\{ \left[(P-P_o)\eta + C_1 G_{\eta'} + C_2(\eta\rho u) \right] \delta\eta \right\} \Bigg|_{X_A}^{X_c} +$$
$$+ \int_A^C \left\{ \left[\eta\eta' P_y - \eta \frac{dP}{dx} + C_1 G_\eta + C_1 G_P P_y + C_2 \frac{d}{dx}(\eta\rho u) - \right. \right.$$
$$\left. \left. - C_1 \frac{d}{dx}(G_{\eta'}) - \frac{d}{dx}(C_2 \eta\rho u) \right] \delta\eta \right\} dx = 0 \tag{62}$$

For arbitrary δX_c, the first term in Eq. (62) must be zero. Eliminating C_1 from this term by introducing Eq. (60), and recalling from Eq. (29) that $h_1 = C_2$ on the wall AC, gives the following result for $h_1(X_c)$ and $C_2(X_c)$.

$$h_1(X_c) = C_2(X_c) = - \frac{(P_c - P_o)}{\rho_c u_c} \left[1 - \frac{\eta_c' \, G_{\eta'}(X_c)}{G(X_c)} \right] \qquad (63)$$

Rearranging the line integral in Eq. (62) and introducing the system momentum equations, Eqs. (2) and (3), gives, for arbitrary $\delta\eta$,

$$\frac{dC_2}{dx} = \frac{du}{dx} - \frac{(P_c - P_o)\eta_c \eta_c'}{G(X_c)} \times \frac{1}{\eta \rho u} \left[\frac{d}{dx} (G_{\eta'}) + \rho u G_P \frac{dv}{dx} - G_\eta \right] \qquad (64)$$

Integrating Eq. (64), using Eq. (63) to evaluate the constant of integration, and recalling from Eq. (29) that $h_1 = C_2$ on AC, the following expression for $h_1[x,\eta(x)]$ along AC is obtained.

$$h_1[x,\eta(x)] = (u - u_c) - \frac{(P_c - P_o)}{\rho_c u_c} \left[1 - \frac{\eta_c' \, G_{\eta'}(X_c)}{G(X_c)} \right] -$$

$$- \frac{(P_c - P_o)\eta_c \eta_c'}{G(X_c)} \int_X^{X_c} \frac{1}{\eta \rho u} \left[\frac{d}{dx} \left(\frac{\partial G}{\partial \eta'}\right) + \rho u \left(\frac{\partial G}{\partial P}\right) \frac{dv}{dx} - \left(\frac{\partial G}{\partial \eta}\right) \right] dx \qquad (65)$$

Thus the Lagrange multiplier $h_1(x,y)$ can be evaluated along AC, giving a boundary condition, in terms of the gasdynamic properties and the general isoperimetric constraint $G(\eta,\eta', P)$, for the determination of the Lagrange multipliers throughout the flow field ABC. Examples of the general isoperimetric constraint are presented in the next section.

E. Examples of the General Isoperimetric Constraint

The general isoperimetric constraint $G(\eta,\eta',P)$ was defined in Eq. (12). The function $G(\eta,\eta',P)$ can be chosen at the discretion of the nozzle designer. Results for constant length, constant surface area, constant arc length, and constant nozzle weight are presented in this section.

For constant nozzle length, Eq. (12) becomes

$$S = \text{Axial Length} = \int_A^C dx = \text{Constant} \tag{66}$$

Hence, the general isoperimetric constraint is given by

$$G(\eta,\eta',P) = 1 \tag{67}$$

Substituting Eq. (67) into Eq. (65) gives the following result for h_1 along AC.

$$h_1[x,\eta(x)] = (u - u_c) - \frac{(P_c-P_o)}{\rho_c u_c} \tag{68}$$

For constant nozzle surface area, Eq. (12) becomes

$$S = \frac{\text{Surface Area}}{2\pi} = \int_A^C (1 + \eta'^2)^{\frac{1}{2}} \eta \, dx = \text{Constant} \tag{69}$$

Hence, the general isoperimetric constraint is given by

$$G(\eta,\eta',P) = (1 + \eta'^2)^{\frac{1}{2}} \eta \tag{70}$$

Substituting Eq. (70) into Eq. (65) gives the following result for h_1 for a constant surface area nozzle.

$$h_1[x,\eta(x)] = (u - u_c) - \frac{(P_c-P_o) \cos^2 \theta_c}{\rho_c u_c} +$$

$$+ (P_c-P_o) \sin\theta_c \int_X^{X_c} \frac{1}{\eta\rho u} \left[\sec \theta - \frac{d}{dx} (\eta \sin \theta)\right] dx \tag{71}$$

For constant nozzle wall arc length, a compromise between constant length and constant surface area, Eq. (12) becomes

$$S = \text{Arc Length} = \int_A^C (1 + \eta'^2)^{\frac{1}{2}} dx = \text{Constant} \tag{72}$$

In this case, the general isoperimetric constraint becomes

$$G(\eta,\eta',P) = (1 + \eta'^2)^{\frac{1}{2}} \tag{73}$$

For this case,

$$h_1[x,\eta(x)] = (u - u_c) - \frac{(P_c-P_o)\cos^2\theta_c}{\rho_c u_c} -$$

$$- (P_c-P_o)\eta_c \sin\theta_c \int_X^{X_c} \frac{1}{\eta\rho u} \left[\frac{d}{dx}(\sin\theta)\right] dx \tag{74}$$

As a final example of the general isoperimetric constraint, consider the case where the weight of the nozzle is assumed to be governed solely by the mechanical stresses in the wall material. If the nozzle weight is held constant, and the wall stress is assumed to be constant, the following expression is obtained for the constraint integral.

$$S = \frac{\sigma_W \times \text{Weight}}{4\pi\rho_W} = \int_A^C (P - P_o)\, \eta^2 (1 + \eta'^2)^{\frac{1}{2}} dx = \text{Constant} \tag{75}$$

The general isoperimetric constraint for this case is

$$G(\eta,\eta',P) = (P - P_o)\eta^2(1 + \eta'^2)^{\frac{1}{2}} \tag{76}$$

Substituting Eq. (76) into Eq. (65) gives the following result for h_1.

$$h_1[x,\eta(x)] = (u - u_c) - \frac{(P_c - P_o)\cos^2\theta_c}{\rho_c u_c} - \frac{\sin\theta_c}{\eta_c} \times$$

$$\times \int_X^{X_c} \frac{1}{\eta\rho u}\left\{\frac{d}{dx}\left[(P-P_o)\eta^2\sin\theta\right] + \rho u\eta^2\sec\theta\,\frac{dv}{dx} - 2(P-P_o)\eta\sec\theta\right\} dx \quad (77)$$

As discussed by Guderley and Armitage,[18] Eq. (75) does not represent a realistic engineering constraint since the wall pressures may become very low, resulting in very thin nozzle walls having very large surface areas. This problem can be overcome by combining this constraint with any of the other three constraints with a penalty coefficient as discussed by Guderley and Armitage.[18]

It is obvious that many more engineering constraints can be postulated, and the results used to evaluate the Lagrange multiplier h_1 along the nozzle wall. The only other effect on the results developed herein is the inclusion of the term uG_pC_1 in Eq. (30). For constraints independent of pressure, this term will always be zero.

F. Summary of the Resulting Equations

In this section, the results of the optimization analysis are summarized. These results are a set of characteristic and compatibility equations for the gasdynamic properties and the Lagrange multipliers valid in region ABC, and a set of boundary conditions for these variables on the boundaries of region ABC. The geometry is illustrated in Fig 1.

Along the boundary AB: The gasdynamic properties u, v, P, ρ, and C_i are known from the characteristics solution of the kernel.

Along the boundary AC: The following boundary conditions were obtained along the nozzle wall.

$$\frac{dy}{dx} = \frac{v}{u} \tag{78}$$

$$h_1[x,\eta(x)] = (u-u_c) - \frac{(P_c-P_o)}{\rho_c u_c}\left[1 - \frac{\eta_c' \, G_{\eta'}(X_c)}{G(X_c)}\right] -$$

$$- \frac{(P_c-P_o)\eta_c\eta_c'}{G(X_c)} \int_X^{X_c} \frac{1}{\eta\rho u}\left[\frac{d}{dx}\left(\frac{\partial G}{\partial \eta'}\right) + \rho u \left(\frac{\partial G}{\partial P}\right)\frac{dv}{dx} - \left(\frac{\partial G}{\partial \eta}\right)\right] dx \tag{79}$$

$$uh_3 - vh_2 + v\eta - \frac{u\eta_c\eta_c' \, (P_c-P_o)}{G(\eta_c,\eta_c', P_c)} G_P = 0 \tag{80}$$

where $G(\eta,\eta',P)$ is the general isoperimetric constraint to be specified by the nozzle designer.

Along the boundary BC: The following boundary conditions were obtained along the exit control characteristic BC.

$$yy'h_1 + (uy' - v)h_2 = 0 \tag{81}$$

$$yh_1 - (uy' - v)h_3 = 0 \tag{82}$$

$$yh_1 - a^2 h_4 = 0 \tag{83}$$

$$g_i = 0 \qquad\qquad i = (1,..,n) \tag{84}$$

Along gas streamlines: The following compatibility equations were found along gas streamlines in region ABC.

$$\frac{dy}{dx} = \frac{v}{u} \tag{85}$$

$$\rho u du + \rho v dv + dP = 0 \tag{86}$$

$$dP - a^2 d\rho = + \frac{1}{u} \sum \psi_i \; dx \tag{87}$$

$$\rho u dC_i = \sigma_i dx \qquad (i = 1,..,n) \tag{88}$$

$$- h_2 du - h_3 dv + y dh_1 + u dh_2 + v dh_3 =$$

$$= K_1 dx + K_2 dy - \frac{1}{\rho u} h_4 \sum \psi_i dx + \frac{1}{\rho u} \sum g_i \sigma_i dx \tag{89}$$

$$(vh_2 - uh_3) dv + \frac{1}{\rho} h_2 \; dP - \frac{1}{\rho} h_4 a^2 u \; (\gamma - 1) d\rho + yu dh_1 - ua^2 dh_4 =$$

$$= \left(- \frac{h_4 a^2 v}{y} - a^2 K_3 + K_4 \right) dx \tag{90}$$

$$u dg_i = J_i dx - h_4 a^2 u a_i d\rho \qquad (i = 1,..,n) \tag{91}$$

<u>Along Mach lines</u>: The following compatibility equations were obtained along Mach lines in region ABC.

$$\frac{dy}{dx} = \tan \; (\theta \pm \alpha) \tag{92}$$

$$a^2 (v du - u dv) \pm \frac{a^2 \cot\alpha}{\rho} dP = (u dy - v dx) \left(\frac{a^2 v}{y} + \frac{1}{\rho} \sum \psi_i \right) \tag{93}$$

$$h_2du + h_3dv + \frac{1}{\rho} h_4 (dP - a^2d\rho) + \sum_{i=1}^{n} g_i dC_i - ydh_1 \mp$$

$$\mp \tan \alpha(vdh_2 - udh_3) = \pm \tan\alpha(K_2dx - K_1dy) \pm$$

$$\pm \frac{1}{a^2} \tan\alpha \; (udy - vdx) \left(K_4 + \frac{1}{\rho} h_4 \sum_{i=1}^{n} \Psi_i \right) \tag{94}$$

In Eqs. (92), (93), and (94), the upper signs refer to left running Mach lines and the lower signs to right running Mach lines.

III. APPLICATION OF THE RESULTS

The application of the results of the present optimization analysis is quite involved. A complete set of characteristic and compatibility equations for the gasdynamic properties and the Lagrange multipliers was obtained. The characteristics are the gas streamlines and the gas Mach lines. The characteristic and compatibility equations for determining the gas properties and the Lagrange multipliers are Eqs. (85) through (94).

Initial conditions for the gasdynamic properties can be determined from a transonic analysis as discussed by Der[22] and Craig.[23] Initial conditions for the Lagrange multipliers h_1 through h_4 and g_i at point C can be determined from Eqs. (79), (80), (81), (83), and (84). Values of these multipliers along AC can be evaluated by employing Eqs. (79), (80), (89), (90), and (91), starting with the known values at point C. As seen from Eq. (84), the Lagrange multipliers g_i are all zero along BC. Note that Eq. (82) relating h_1 and h_3 along the exit control characteristic BC is not needed in the determination of the initial conditions. This equation can be employed as a check to determine whether or not a given contour is the desired optimum contour.

A method for the direct application of the results of this analysis for the determination of optimum thrust nozzle contours is not presented. However, the results can be applied in a straightforward manner to determine if a given nozzle contour is the desired optimum contour. For a given contour, the entire gasdynamic flow field can be determined by applying the method of characteristics. The initial conditions for the Lagrange multipliers along the wall AC and along the exit characteristic BC can be determined as discussed above. The remainder of the analysis involves the construction of a characteristic network as illustrated in Fig. 2.

Starting near the nozzle exit at point 1, the initial data known along the contour AC can be employed, along with Eq. (94) which is valid along the two Mach lines intersecting at point 2, and Eqs. (81) and (83) which are valid along Mach line BC, to determine the Lagrange multipliers h_1 through h_4 at point 2. The values of h_1 through h_4 and g_i can be found at point 3 by applying Eq. (94) along the two Mach lines intersecting at point 3 and Eqs. (89), (90), and (91) along the gas streamline from point 2 to 3. Point 4 can be found in the same manner as point 2 was found. By continuing this step by step procedure the Lagrange multipliers h_1 through h_4 and g_i can be determined throughout region ABC.

During the above procedure, Eq. (82) was not employed. This relationship can thus be utilized as a means of checking whether or not the selected contour is indeed the optimum contour. Thus, along BC, the error parameter E can be evaluated.

$$E = yh_1 - (uy' - v)h_3 \tag{95}$$

If E is everywhere zero along BC, then the contour satisfies all the requirements of the variational problem and is indeed the optimum contour.

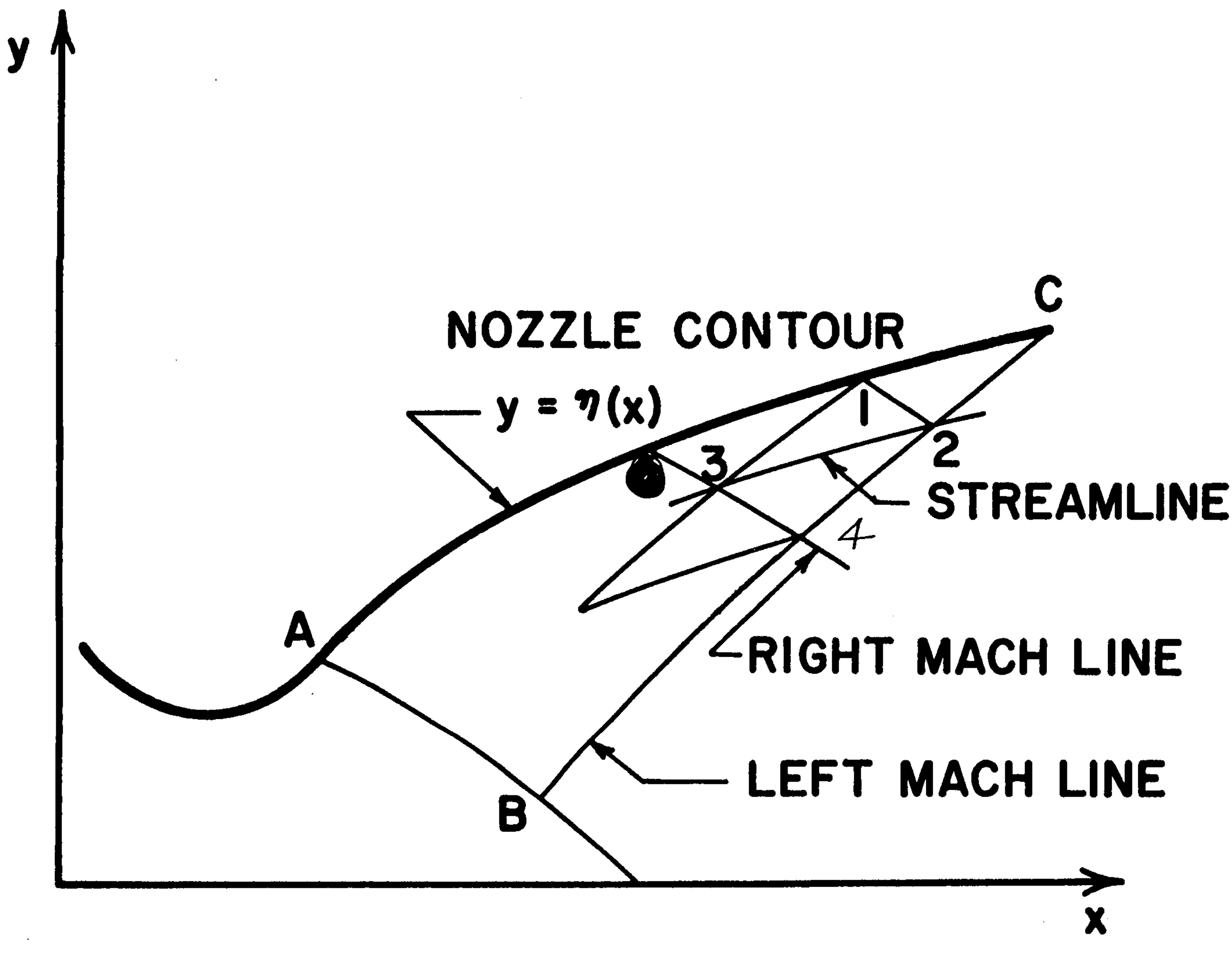

FIGURE 2. CHARACTERISTIC NETWORK

Otherwise, the contour must be altered by a relaxation technique to approach the desired optimum contour.

Guderley and Armitage[18] present a relaxation technique which was applied to their results, which are similar to the present results. Although the present problem is more involved, a similar relaxation technique can be developed to permit the determination of optimum thrust nozzle contours for chemically reacting gas flows.

IV. CONCLUSIONS

An analysis was presented for the optimization of nozzle contours to give maximum thrust for chemically reacting flows. The solution is subject to the constraints of fixed subsonic and transonic nozzle geometry, and a general isoperimetric constraint imposed along the wall in the supersonic flow regime. The solution was obtained in the form of a set of partial differential equations for the Lagrange multipliers of the optimization problem. A complete set of characteristic and compatibility equations for the gasdynamic properties and the Lagrange multipliers was obtained. Boundary conditions for the Lagrange multipliers were obtained from the optimization analysis in the form of a set of algebraic equations valid along the boundaries of the flow field. A method was presented for employing the results to determine whether or not a given nozzle contour is actually an optimum contour. By employing a relaxation technique in conjunction with the aforementioned method, a procedure can be developed with which the desired optimum contour can be obtained. The application of such a technique would permit the rocket nozzle designer to obtain the best possible performance subject to the constraints of each individual application.

V. NOMENCLATURE

English Symbols

a	frozen speed of sound
a_i	function of specific heats defined by Eq. (24)
C_i	species mass fraction
C_p	constant pressure specific heat
C_{pi}	constant pressure specific heat of species i
C_v	constant volume specific heat
C_{vi}	constant volume specific heat of species i
C_1	Lagrange multiplier
C_2	Lagrange multiplier
E	error parameter defined by Eq. (95)
F	thrust parameter to be maximized, defined by Eq. (11)
g_i	Lagrange multipliers $(i=1,\ldots,n)$
G	general isoperimetric constraint defined by Eq. (12)
h_i	enthalpy of species i
h_i^o	heat of formation of species i
h_j	Lagrange multipliers $(j=1,\ldots,4)$
J_i	nonhomogeneous terms in Eqs. (39)
K_j	nonhomogeneous terms in Eqs. (35) through (38)
K_{fr}	forward reaction rate constant of reaction r
K_{rr}	reverse reaction rate constant of reaction r

L_j	partial differential equation operator defined by Eq. (14)
M_i	partial differential equation operator defined by Eq. (15)
n	number of chemical species i
N	number of chemical reactions r
P	pressure
P_o	ambient pressure
R	gas constant
R_i	gas constant of species i
S	general isoperimetric constraint integral defined by Eq. (12)
t	time
T	temperature
u	x-direction velocity component
v	y-direction velocity component
W	molecular weight
W_i	molecular weight of species i
x	coordinate along nozzle axis
X_c	x coordinate of nozzle exit point C
y	coordinate normal to nozzle axis

Greek Symbols

α	Mach angle, $\alpha = \sin^{-1}(1/M)$
γ	specific heat ratio
$\delta(\ )$	first variation of a quantity
$\eta(x)$	optimized nozzle contour
θ	flow angle, $\theta = \tan^{-1}(v/u)$
ν'_{ir}	stoichiometric coefficients of reactants

ν''_{ir}	stoichiometric coefficients of products
ρ	density
ρ_w	density of nozzle wall material
σ_i	chemical species source function
σ_w	stress of nozzle wall material
ψ_i	function of thermodynamic properties defined by Eq. (7)

Subscripts

c	property evaluated at nozzle exit point C
i	index denoting species i (i=1,...,n)
j	index denoting species j (j=1,...,n)
k	index denoting species k (k=1,...,n)
r	index denoting reaction r (r=1,...,N)

Other

$\frac{d}{dx}$	total derivative with respect to x
$\frac{\partial}{\partial x}$	partial derivative with respect to x
$\frac{\partial}{\partial y}$	partial derivative with respect to y
$(\ )_x$	partial derivative with respect to x
$(\ )_y$	partial derivative with respect to y
$(\ )_\phi$	partial derivative with respect to ϕ ($\phi = \eta, \eta'$, or P)
$\frac{dy}{dx}$	slope of a line in x-y plane

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APPENDIX A

GOVERNING EQUATIONS FOR CHEMICALLY REACTING FLOWS

The governing equations for the axisymmetric flow of a chemically reacting gas in the absence of transport phenomena and body forces are given in references 21, 22 and 23. These equations are the usual equations for conservation of mass, momentum, and energy, the thermal equation of state, and the caloric equation of state. Generally, these equations are presented in the natural coordinate system consisting of an axis along a streamline and an axis normal to the streamline. In that coordinate system, (2+n) of the (4+n) governing partial differential equations reduce to total differential equations along a streamline, thus leaving only two partial differential equations to be solved by the method of characteristics. In the present optimization analysis, the aforementioned simplification is not advantageous, since the governing equations must be solved simultaneously with the set of partial differential equations governing the Lagrange multipliers of the optimization problem. The form of the governing equations employed in the present analysis is developed in the following discussion.

From reference (22), the following equations are obtained.

$$\frac{D\rho}{Dt} + \rho \operatorname{div} \overline{V} = 0 \qquad \text{(A-1)}$$

$$\rho \frac{D\overline{V}}{Dt} + \text{grad } P = 0 \tag{A-2}$$

$$\rho \frac{Dh}{Dt} - \frac{DP}{Dt} = 0 \tag{A-3}$$

$$\rho \frac{DC_i}{Dt} = \sigma_i \qquad (i=1,..,n) \tag{A-4}$$

$$P = \rho T \sum_{i=1}^{n} C_i R_i \tag{A-5}$$

$$h = \sum_{i=1}^{n} C_i h_i \tag{A-6}$$

$$h_i = \int_{To}^{T} C_{pi} T + h_i^o \qquad (i=1,..,n) \tag{A-7}$$

When expanded into a cylindrical coordinate system, Eqs. (A-1) through (A-4) result in (4+n) partial differential equations for the (5+n) variables u, v, P, ρ, h and C_i. In order to apply the method of characteristics to this system, the enthalpy h appearing in Eq. (A-3) will be eliminated by using Eqs. (A-5), (A-6), and (A-7). Consider the term h_x arising from Eq. (A-3).

$$h_x = \sum_{i=1}^{n} h_i (C_i)_x + \sum_{i=1}^{n} C_i (h_i)_x \tag{A-8}$$

From Eq. (A-7), assuming constant specific heats,

$$(h_i)_x = C_{pi} T_x \tag{A-9}$$

From Eq. (A-5),

$$T_x = \frac{T}{P} P_x - \frac{T}{\rho} \rho_x - \frac{T}{R} \sum_{i=1}^{n} R_i (C_i)_x \tag{A-10}$$

Substituting Eqs. (A-9) and (A-10) into Eq. (A-8) gives the following result.

$$h_x = \frac{C_p T}{P} P_x - \frac{C_p T}{\rho} \rho_x + \sum_{i=1}^{n} \left(h_i - \frac{C_p T R_i}{R}\right) (C_i)_x \tag{A-11}$$

In a similar manner, h_y is given by

$$h_y = \frac{C_p T}{P} P_y - \frac{C_p T}{\rho} \rho_y + \sum_{i=1}^{n} \left(h_i - \frac{C_p T R_i}{R}\right) (C_i)_y \tag{A-12}$$

Substituting Eqs. (A-11) and (A-12) into the energy equation, Eq. (A-3), gives the following result.

$$\frac{C_p T}{P} \frac{DP}{Dt} - \frac{C_p T}{\rho} \frac{D\rho}{Dt} + \sum_{i=1}^{n} \left(h_i - \frac{C_p T R_i}{R}\right) \frac{DC_i}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} = 0 \tag{A-13}$$

Multiplying Eq. (A-13) by $(\gamma-1)\rho$ yields

$$\frac{DP}{Dt} - a^2 \frac{D\rho}{Dt} + (\gamma-1) \sum_{i=1}^{n} \left(h_i - \frac{C_p T R_i}{R}\right)\rho \frac{DC_i}{Dt} = 0 \tag{A-14}$$

Substituting the species continuity equation, Eq. (A-4), into Eq. (A-14) yields

$$\frac{DP}{Dt} - a^2 \frac{D\rho}{Dt} = \sum_{i=1}^{n} \psi_i \tag{A-15}$$

where the function ψ_i is defined as follows.

$$\sum_{i=1}^{n} \psi_i = \sum_{i=1}^{n} \left[\gamma R_i T - (\gamma-1)h_i\right] \sigma_i \tag{A-16}$$

In summary, the governing differential equations for the flow of a chemically reacting gas are Eqs. (A-1), (A-2), (A-15), and (A-4). When expanded into a cylindrical coordinate system, these equations have the following form.

$$\rho u_x + \rho v_y + u\rho_x + v\rho_y = -\frac{\rho v}{y} \tag{A-17}$$

$$\rho u u_x + \rho v u_y + P_x = 0 \tag{A-18}$$

$$\rho u v_x + \rho v v_y + P_y = 0 \tag{A-19}$$

$$uP_x + vP_y - a^2 u\rho_x - a^2 v\rho_y = \sum_{i=1}^{n} \psi_i \tag{A-20}$$

$$\rho u(C_i)_x + \rho v(C_i)_y = \sigma_i \qquad (i=1,..,n) \tag{A-21}$$

APPENDIX B

ANALYSIS OF VARIATIONS OF GAS PROPERTIES

In this section, variations will be taken in the gas properties $u(x,y)$, $v(x,y)$, $P(x,y)$, $\rho(x,y)$ and $C_i(x,y)$ $(i=1,..,n)$, along the contour $\eta(x)$ and throughout the flow field ABC. In order to take variations in properties which appear in differential form, the following relationship will be employed.

$$\delta(f_x) = \frac{\partial}{\partial x}(\delta f) \tag{B-1}$$

Employing the above relationship and taking variations of all gas properties in Eq. (18) yields the following result.

$$\int_A^C \left[\eta\eta'\delta P + C_1 G_p \delta P + C_2(x)\eta\rho(\eta'\delta u - \delta v)\right]dx +$$

$$+ \iint_{ABC} \left\{ h_1(x,y) \left[\frac{\partial}{\partial x}\delta(y\rho u) + \frac{\partial}{\partial y}\delta(y\rho v)\right] + \right.$$

$$+ h_2(x,y) \left[\delta(\rho u u_x) + \delta(\rho v u_y) + \frac{\partial}{\partial x}\delta P\right] +$$

$$+ h_3(x,y) \left[\delta(\rho u v_x) + \delta(\rho v v_y) + \frac{\partial}{\partial y}\delta P\right] +$$

$$+ h_4(x,y) \left[\delta(uP_x) + \delta(vP_y) - \delta(a^2 u\rho_x) - \delta(a^2 v\rho_y) - \sum_{i=1}^{n}\delta\psi_i\right] +$$

$$\left. + \sum_{i=1}^{n} g_i(x,y) \left[\delta\{\rho u(C_i)_x\} + \delta\{\rho v(C_i)_y\} - \delta\sigma_i\right] \right\} dxdy = 0 \tag{B-2}$$

From here on, the terms $C_2(x)$, $h_1(x,y)$, etc. will be denoted by C_2, h_1, etc. in order to simplify the appearance of the equations.

The surface integral over the region ABC can be simplified by applying Green's theorem for the plane which can be stated as follows. If $M(x,y)$, $N(x,y)$, $\partial M/\partial y$, and $\partial N/\partial x$ are continuous, single-valued functions over a closed region R bounded by the closed curve C, then

$$\int\int_R \left(\frac{\partial N}{\partial x} - \frac{\partial M}{\partial y}\right) dxdy = \int_C (Mdx + Ndy) \qquad \text{(B-3)}$$

The double integral is taken over the given region R, and the curve C is described in a direction such that the region R is to the left when traveling in a positive direction around the curve. In order to simplify the application of Green's theorem to Eq. (B-2), the integral over the region ABC, in Eq. (B-2) can be considered to be represented by the following expression.

$$(G+H) + (J+K+P) + (L+M+Q) + (R+S+T+U+V) + (X+Y+Z) \qquad \text{(B-4)}$$

where

$$G = \int\int_{ABC} h_1 \frac{\partial}{\partial x} \delta(y\rho u)dxdy \qquad \text{(B-5)}$$

and the remaining terms follow in sequence from Eq. (B-2). Green's theorem can then be applied to each of the terms in Eq. (B-4) as follows. Consider the terms G and H.

$$G = \int\int_{ABC} h_1 \frac{\partial}{\partial x} \delta(y\rho u)\,dxdy \tag{B-6}$$

$$G = \int\int_{ABC} \{\frac{\partial}{\partial x} [h_1 \delta(y\rho u)] - \delta(y\rho u) \ (h_1)_x\}dxdy \tag{B-7}$$

$$H = \int\int_{ABC} h_1 \frac{\partial}{\partial y} \delta(y\rho v)\,dxdy \tag{B-8}$$

$$H = \int\int_{ABC} \{\frac{\partial}{\partial y} [h_1 \delta(y\rho v)] - \delta(y\rho v) \ (h_1)_y\}dxdy \tag{B-9}$$

In Eqs. (B-7) and (B-9), let

$$M = - h_1 \delta(y\rho v) \tag{B-10}$$

$$N = h_1 \delta(y\rho u) \tag{B-11}$$

Adding Eqs. (B-7) and (B-9), and applying Green's theorem gives

$$(G+H) = \left\{\int_A^B + \int_B^C + \int_C^A\right\} \left[- h_1 \delta(y\rho v)dx + h_1 \delta(y\rho u)dy\right] + \\ + \int\int_{ABC} \{- \delta(y\rho u)(h_1)_x - \delta(y\rho v)(h_1)_y\}dxdy \tag{B-12}$$

Consider the terms J and K.

$$J = \int\int_{ABC} h_2 \delta(\rho u u_x)\,dxdy \tag{B-13}$$

$$J = \int\int_{ABC} \{h_2 \delta(\rho u) u_x + h_2 \rho u \frac{\partial}{\partial x} \delta u\}dxdy \tag{B-14}$$

Note that

$$\frac{\partial}{\partial x}(h_2\rho u\delta u) = h_2\rho u \frac{\partial}{\partial x}\delta u + \delta u(h_2\rho u)_x \tag{B-15}$$

Substituting Eq. (B-15) into Eq. (B-14) gives

$$J = \int\int_{ABC}\{h_2\delta(\rho u)u_x + (h_2\rho u\delta u)_x - \delta u(h_2\rho u)_x\}dxdy \tag{B-16}$$

Performing analogous operations on the term K gives

$$K = \int\int_{ABC}\{h_2\delta(\rho v)u_y + (h_2\rho v\delta u)_y - \delta u(h_2\rho v)_y\}dxdy \tag{B-17}$$

In Eqs. (B-16) and (B-17), let

$$M = -\ h_2\rho v\delta u \tag{B-18}$$

$$N = \ h_2\rho u\delta u \tag{B-19}$$

Adding Eqs. (B-16) and (B-17), and applying Green's theorem gives

$$(J+K) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left[-\ h_2\rho v\delta u dx + h_2\rho u\delta u dy\right] +$$

$$+ \int\int_{ABC}\{h_2\delta(\rho u)u_x + h_2\delta(\rho v)u_y - \delta u(h_2\rho u)_x - \delta u(h_2\rho v)_y\}dxdy \tag{B-20}$$

Treating L and M in the same manner in which J and K were modified results in the following expression.

$$(L+M) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left[- h_3\rho v\delta v dx + h_3\rho u\delta v dy\right] +$$

$$+ \iint_{ABC}\{h_3\delta(\rho u)v_x + h_3\delta(\rho v)v_y - \delta v(h_3\rho u)_x - \delta v(h_3\rho v)_y\}dxdy \quad \text{(B-21)}$$

Performing similar operations on P and Q yields

$$(P+Q) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left[- h_3\delta P dx + h_2\delta P dy\right] +$$

$$+ \iint_{ABC}\{- \delta P(h_2)_x - \delta P(h_3)_y\}dxdy \quad \text{(B-22)}$$

Combining R and S in the same manner gives

$$(R+S) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left[- h_4 v\delta P dx + h_4 u\delta P dy\right] +$$

$$+ \iint_{ABC}\{h_4\delta u P_x + h_4\delta v P_y - \delta P(h_4 u)_x - \delta P(h_4 v)_y\}dxdy \quad \text{(B-23)}$$

Performing similar operations on T and U results in

$$(T+U) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left[h_4 a^2 v\delta\rho dx - h_4 a^2 u\delta\rho dy\right] +$$

$$+ \iint_{ABC}\{- h_4\delta(a^2u)\rho_x - h_4\delta(a^2v)\rho_y + \delta\rho(h_4a^2u)_x +$$

$$+ \delta\rho(h_4a^2v)_y\}dxdy \quad \text{(B-24)}$$

Combining X and Y in the same manner gives

$$(X+Y) = \left\{\int_A^B + \int_B^C + \int_C^A\right\}\left\{\sum_{i=1}^{n}\left[- g_i\rho v\delta C_i dx + g_i\rho u\delta C_i dy\right]\right\} +$$

$$+ \iint_{ABC}\left\{\sum_{i=1}^{n}\left[g_i(C_i)_x\delta(\rho u) + g_i(C_i)_y\delta(\rho v) - \delta C_i(g_i\rho u)_x - \right.\right.$$

$$\left.\left. - \delta C_i(g_i\rho v)_y\right]\right\} dxdy \qquad \text{(B-25)}$$

The terms V and Z are non-homogeneous terms not involving partial derivatives. At this point, these terms will be treated in functional form without specifying the exact form of the function. Thus,

$$V = \iint_{ABC}\{- h_4 \sum_{i=1}^{n}\delta\psi_i\}dxdy \qquad \text{(B-26)}$$

The term ψ_i is assumed to be a function of P, ρ, and C_k only. Thus,

$$V = \iint_{ABC} h_4\left\{- \delta P \sum_{i=1}^{n}\psi_{iP} - \delta\rho \sum_{i=1}^{n}\psi_{i\rho} - \right.$$

$$\left. - \sum_{i=1}^{n}\left[\sum_{k=1}^{n}(\psi_k)_{C_i}\right]\delta C_i\right\} dxdy \qquad \text{(B-27)}$$

In a similar manner, the following result is obtained for Z.

$$Z = \iint_{ABC}\left\{- \delta P \sum_{i=1}^{n} g_i\sigma_{iP} - \delta\rho \sum_{i=1}^{n} g_i\sigma_{i\rho} - \right.$$

$$\left. - \sum_{i=1}^{n}\left[\sum_{k=1}^{n} g_k(\sigma_k)_{C_i}\right]\delta C_i\right\} dxdy \qquad \text{(B-28)}$$

The term δa^2 appears in Eq. (B-24). This term can be eliminated by considering the equation for the frozen speed of sound in a perfect gas.

$$a^2 = \frac{\gamma P}{\rho} = \frac{C_p P}{C_v \rho}$$

$$\delta a = \frac{a^2}{C_p} \delta C_p - \frac{a^2}{C_v} \delta C_v + \frac{a^2}{P} \delta P - \frac{a^2}{\rho} \delta \rho \qquad \text{(B-29)}$$

$$C_p = \sum_{i=1}^{n} C_{pi} C_i \qquad \text{(B-30)}$$

$$\delta C_p = \sum_{i=1}^{n} C_{pi} \delta C_i \qquad \text{(B-31)}$$

$$C_v = \sum_{i=1}^{n} C_{vi} C_i \qquad \text{(B-32)}$$

$$\delta C_v = \sum_{i=1}^{n} C_{vi} \delta C_i \qquad \text{(B-33)}$$

Substituting Eqs. (B-31) and (B-33) into Eq. (B-29) gives the following result for δa^2.

$$\delta a^2 = \frac{a^2}{P} \delta P - \frac{a^2}{\rho} \delta \rho + a^2 \sum_{i=1}^{n} a_i \delta C_i \qquad \text{(B-34)}$$

where

$$a_i = \frac{1}{C_p} (C_{pi} - \gamma C_{vi}) \qquad \text{(B-35)}$$

Equation (B-24) also contains partial derivatives of a^2 with respect to x and y. These derivatives can be obtained in the same manner as Eq.

(B-34) was developed. Thus,

$$a_x^2 = \frac{a^2}{P} P_x - \frac{a^2}{\rho} \rho_x + a^2 \sum_{i=1}^{n} a_i (C_i)_x \tag{B-36}$$

$$a_y^2 = \frac{a^2}{P} P_y - \frac{a^2}{\rho} \rho_y + a^2 \sum_{i=1}^{n} a_i (C_i)_y \tag{B-37}$$

Note that in region ABC

$$\delta(y\rho u) = y\rho\delta u + yu\delta\rho \tag{B-38}$$

$$\delta(y\rho v) = y\rho\delta v + \rho v\delta\rho \tag{B-39}$$

Substituting all of the above results into Eq. (B-2) yields the following expression. Note that the direction of the line integrals has been reversed by interchanging the limits of integration and multiplying the integrands by (-1), resulting in no net change in the values of the integrals.

$$\left.\begin{aligned}
&\int_A^C \left\{\eta\eta'\delta P + C_1 G_p \delta P + C_2 \eta\rho(\eta'\delta u - \delta v)\right\} dx + \\
&+ \left\{\int_A^C - \int_B^C - \int_A^B\right\} \left\{h_1 y\rho\delta v + h_1 yv\delta\rho + h_2 \rho v\delta u + h_3 \rho v\delta v + \right. \\
&\qquad\qquad \left. + h_3 \delta P + h_4 v\delta P - h_4 a^2 v\delta\rho + \rho v \sum_{i=1}^{n} g_i \delta C_i\right\} dx - \\
&- \left\{\int_A^C - \int_B^C - \int_A^B\right\} \left\{h_1 y\rho\delta u + h_1 yu\delta\rho + h_2 \rho u\delta u + h_3 \rho u\delta v + \right.
\end{aligned}\right\} \tag{B-40}$$

$$+ h_2\delta P + h_4 u\delta P - h_4 a^2 u\delta\rho + \rho u \sum_{i=1}^{n} g_i \delta C_i \Big\} \, dy + \qquad \text{(B-40)}$$

$$+ \int\int_{ABC} \Big\{ \Big[- y\rho(h_1)_x + h_2\rho u_x - (h_2\rho u)_x - (h_2\rho v)_y + h_3\rho v_x +$$

$$+ h_4 P_x - h_4 a^2 \rho_x + \rho \sum_{i=1}^{n} g_i (C_i)_x \Big] \delta u +$$

$$+ \Big[- y\rho(h_1)_y + h_2\rho u_y + h_3\rho v_y - (h_3\rho u)_x - (h_3\rho v)_y +$$

$$+ h_4 P_y - h_4 a^2 \rho_y + \rho \sum_{i=1}^{n} g_i (C_i)_y \Big] \delta v +$$

$$+ \Big[- h_4 \frac{a^2}{P} (u\rho_x + v\rho_y) - (h_2)_x - (h_3)_y - (h_4 u)_x - (h_4 v)_y -$$

$$- h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i \sigma_{iP} \Big] \delta P +$$

$$+ \Big[- yu(h_1)_x - yv(h_1)_y + h_2 u u_x + h_2 v u_y + h_3 u v_x + h_3 v v_y +$$

$$+ a^2 (h_4 u)_x + a^2 (h_4 v)_y +$$

$$+ h_4 u a^2 \Big\{ \sum_{i=1}^{n} a_i (C_i)_x + \frac{1}{P} P_x - \frac{1}{\rho} \rho_x \Big\} +$$

$$+ h_4 v a^2 \Big\{ \sum_{i=1}^{n} a_i (C_i)_y + \frac{1}{P} P_y - \frac{1}{\rho} \rho_y \Big\} +$$

$$+ u \sum_{i=1}^{n} g_i (C_i)_x + v \sum_{i=1}^{n} g_i (C_i)_y -$$

$$- h_4 \sum_{i=1}^{n} \psi_{i\rho} - \sum_{i=1}^{n} g_i \sigma_{i\rho} \Big] \delta\rho + \qquad \text{(B-40)}$$

$$+ \sum_{i=1}^{n} \left[- h_4 a^2 a_i (u\rho_x + v\rho_y) - (g_i \rho u)_x - (g_i \rho v)_y - \right.$$

$$\left. - h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} - \sum_{k=1}^{n} g_k (\sigma_k)_{C_i} \right] \delta C_i \Bigg\} dxdy = 0 \Bigg] \qquad \text{(B-40)}$$

Consider first the line integrals appearing in Eq. (B-40). Note that along AC

$$\int_A^C f(y)dy = \int_A^C f[\eta(x)]\eta' dx \qquad \text{(B-41)}$$

Substituting Eq. (B-41) into Eq. (B-40), and noting that the line integrals must equal zero independently of the surface integrals for arbitrary variations in the gas properties, the following equations are obtained.

$$\int_A^C \Bigg\{ \left[C_2 \eta \rho \eta' + h_2 \rho v - h_2 \rho u \eta' - h_1 \eta \rho \eta' \right] \delta u +$$

$$+ \left[- C_2 \eta \rho + h_3 \rho v + h_1 \eta \rho - h_3 \rho u \eta' \right] \delta v +$$

$$+ \left[\eta \eta' + h_3 + h_4 v - h_2 \eta' - h_4 u \eta' + C_1 G_P \right] \delta P +$$

$$+ \left[- h_4 a^2 v + h_1 \eta v + h_4 a^2 u \eta' - h_1 \eta u \eta' \right] \delta \rho$$

$$+ \sum_{i=1}^{n} \left[\rho v g_i - \rho u \eta' g_i \right] \delta C_i \Bigg\} dx = 0 \qquad \text{(B-42)}$$

$$\left\{\int_B^C + \int_A^B\right\}\left\{\left[h_2\rho v dx - h_2\rho u dy - h_1 y\rho dy\right]\delta u + \right.$$

$$+ \left[h_3\rho v dx - h_3\rho u dy - h_1 y\rho dx\right]\delta v +$$

$$+ \left[h_3 dx - h_2 dy + h_4 v dx - h_4 u dy\right]\delta P +$$

$$+ \left[- h_4 a^2 v dx + h_1 y v dx + h_4 a^2 u dy - h_1 y u dy\right]\delta\rho +$$

$$\left. + \sum_{i=1}^{n} \left[\rho v g_i dx - \rho u g_i dy\right]\delta C_i \right\} = 0 \qquad \text{(B-43)}$$

Since the integral in Eq. (B-42) must equal zero for arbitrary values of δu, δv, δP, $\delta\rho$, and δC_i, the coefficients of these variations must equal zero identically, resulting in the following equations respectively which must be valid along AC.

$$h_1[x,\eta(x)] = C_2(x) \qquad \text{(B-44)}$$

$$h_1[x,\eta(x)] = C_2(x) \qquad \text{(B-45)}$$

$$uh_3 - vh_2 + v\eta + uC_1G_p = 0 \qquad \text{(B-46)}$$

$$0 = 0 \qquad \text{(B-47)}$$

$$0 = 0 \qquad \text{(B-48)}$$

Thus, the two independent relationships given by Eqs. (B-44) and (B-46) must apply along the nozzle contour AC.

Since no variations in gas properties are allowed along AB, the line integral along that curve will already be zero and no new conditions result. However, the variations along BC are arbitrary, thus requiring the coefficients of the variations to be zero, resulting in the following equations respectively which must be valid along BC.

$$h_2 \rho v dx - h_2 \rho u dy - h_1 y \rho dy = 0 \tag{B-49}$$

$$h_3 \rho v dx - h_3 \rho u dy + h_1 y \rho dx = 0 \tag{B-50}$$

$$h_3 dx - h_2 dy + h_4 v dx - h_4 \overset{u}{\cancel{y}} dy = 0 \tag{B-51}$$

$$- h_4 a^2 v dx + h_1 y v dx + h_4 a^2 u dy - h_1 y u dy = 0 \tag{B-52}$$

$$g_i (u dy - v dx) = 0 \qquad (i=1,\ldots,n) \tag{B-53}$$

Solving these equations simutaneously gives the following equivalent relationships.

$$y y' h_1 + (u y' - v) h_2 = 0 \tag{B-54}$$

$$y h_1 - (u y' - v) h_3 = 0 \tag{B-55}$$

$$y h_1 - a^2 h_4 = 0 \tag{B-56}$$

$$y h_1 - a^2 h_4 = 0 \tag{B-57}$$

$$g_i(uy' - v) = 0 \qquad (i=1,..,n) \qquad \text{(B-58)}$$

Thus, the four independent relationships expressed by Eqs. (B-54), (B-55), (B-56), and (B-58) must apply along the left running Mach line BC.

Returning to the surface integral appearing in Eq. (B-40), the variations in gas properties must be arbitrary over the region of integration. Hence, the coefficients of the variations must be identically zero, resulting in the following partial differential equations.

$$h_2\rho u_x + h_3\rho v_x - h_2[(\rho u)_x + (\rho v)_y] + h_4(P_x - a^2\rho_x) - $$
$$- y\rho(h_1)_x - \rho u(h_2)_x - \rho v(h_2)_y + \rho \sum_{i=1}^{n} g_i(C_i)_x = 0 \qquad \text{(B-59)}$$

$$h_2\rho u_y + h_3\rho v_y - h_3[(\rho u)_x + (\rho v)_y] + h_4(P_y - a^2\rho_y) - $$
$$- y\rho(h_1)_y - \rho u(h_3)_x - \rho v(h_3)_y + \rho \sum_{i=1}^{n} g_i(C_i)_y = 0 \qquad \text{(B-60)}$$

$$- (h_2)_x - (h_3)_y - (h_4 u)_x - (h_4 v)_y - h_4 \frac{a^2}{P} (u\rho_x + v\rho_y) - $$
$$- h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i\sigma_{iP} = 0 \qquad \text{(B-61)}$$

$$\left.\begin{aligned} & h_2(uu_x + vu_y) + h_3(uv_x + vv_y) + h_4a^2(u_x + v_y) + \\ & + h_4ua^2 \left[\frac{1}{P} P_x + \sum_{i=1}^{n} a_i(C_i)_x\right] + h_4va^2 \left[\frac{1}{P} P_y + \sum_{i=1}^{n} a_i(C_i)_y\right] + \\ & + u \sum_{i=1}^{n} g_i(C_i)_x + v \sum_{i=1}^{n} g_i(C_i)_y - yu(h_1)_x - yv(h_1)_y + \end{aligned}\right\} \qquad \text{(B-62)}$$

$$+ a^2 u(h_4)_x + a^2 v(h_4)_y - h_4 \sum_{i=1}^{n} \psi_{i\rho} - \sum_{i=1}^{n} g_i \sigma_{i\rho} = 0 \tag{B-62}$$

$$g_i[(\rho u)_x + (\rho v)_y] + h_4 a^2 a_i (u\rho_x + v\rho_y) + \rho u(g_i)_x + \rho v(g_i)_y +$$

$$+ h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} + \sum_{k=1}^{n} g_k (\sigma_k)_{C_i} = 0 \qquad (i=1,..,n) \tag{B-63}$$

Equations (B-59) and (B-60) can be simplified by employing the gas continuity equation, Eq. (1).

$$[(\rho u)_x + (\rho v)_y] = - \frac{\rho v}{y} \tag{B-64}$$

Thus, Eqs. (B-59) and (B-60), after multiplication by $(-1/\rho)$, become

$$- h_2 u_x - h_3 v_x - h_4 \frac{1}{\rho} (P_x - a^2 \rho_x) + y(h_1)_x + u(h_2)_x +$$

$$+ v(h_2)_y - \sum_{i=1}^{n} g_i (C_i)_x = K_1 \tag{B-65}$$

$$K_1 = h_2 \frac{v}{y} \tag{B-66}$$

$$- h_2 u_y - h_3 v_y - h_4 \frac{1}{\rho} (P_y - a^2 \rho_y) + y(h_1)_y + u(h_3)_x +$$

$$+ v(h_3)_y - \sum_{i=1}^{n} g_i (C_i)_y = K_2 \tag{B-67}$$

$$K_2 = h_3 \frac{v}{y} \tag{B-68}$$

Equation (B-61) can be written in the following form.

$$h_4 u_x + h_4 v_y + h_4 \frac{a^2}{P} (u\rho_x + v\rho_y) + (h_2)_x + (h_3)_y +$$

$$+ u(h_4)_x + v(h_4)_y = K_3 \qquad \text{(B-69)}$$

$$K_3 = - h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i \sigma_{iP} \qquad \text{(B-70)}$$

Next, to simplify Eq. (B-62), recall the system momentum equations, Eqs. (2) and (3).

$$(uu_x + vu_y) = - \frac{1}{\rho} P_x \qquad \text{(B-71)}$$

$$(uv_x + vv_y) = - \frac{1}{\rho} P_y \qquad \text{(B-72)}$$

Multipling Eq. (B-69) by $- a^2$, adding the result to Eq. (B-62), substituting Eqs. (B-71) and (B-72), introducing the system energy equation, Eq. (4), and the species continuity equation, Eq. (5), the following result is obtained.

$$\frac{h_2}{\rho} P_x + \frac{h_3}{\rho} P_y + yu(h_1)_x + yv(h_1)_y + a^2(h_2)_x + a^2(h_3)_y = K_4 \qquad \text{(B-73)}$$

$$K_4 = \frac{h_4 a^2}{P} \sum_{i=1}^{n} \psi_i - h_4 \sum_{i=1}^{n} (a^2 \psi_{iP} + \psi_{i\rho}) - \sum_{i=1}^{n} g_i (a^2 \sigma_{iP} + \sigma_{i\rho}) +$$

$$+ \frac{1}{\rho} \sum_{i=1}^{n} (h_4 a^2 a_i + g_i) \sigma_i \qquad \text{(B-74)}$$

Substituting the continuity equation, Eq. (1), into Eq. (B-63) yields the following result.

$$h_4 a^2 a_i(u\rho_x + v\rho_y) + \rho u(g_i)_x + \rho v(g_i)_y = J_i \qquad (i=1,..,n) \qquad \text{(B-75)}$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} - \sum_{k=1}^{n} g_k(\sigma_k)_{C_i} \qquad (i=1,..,n) \qquad \text{(B-76)}$$

Equations (1) through (5), together with Eqs. (B-65), (B-67), (B-69), (B-73) and (B-75), constitute a system of (8+2n) equations for determining the (8+2n) variables u, v. P, ρ, C_i, h_1, h_2, h_3, h_4, and g_i. As shown in Appendix E, these equations form a system of quasi-linear, non-homogeneous, first order partial differential equations of the hyperbolic type. Thus, the system can be replaced by an equivalent system of characteristic and compatibility equations, which are total differential equations of the first order. The following characteristic system was obtained in Appendix E. Along gas streamlines,

$$\frac{dy}{dx} = \frac{v}{u} \qquad \text{(B-77)}$$

$$\rho u du + \rho v dv + dP = 0 \qquad \text{(B-78)}$$

$$dP - a^2 d\rho = \frac{1}{u} \sum_{i=1}^{n} \psi_i \, dx \qquad \text{(B-79)}$$

$$\rho u dC_i = \sigma_i dx \qquad (i=1,..,n) \qquad \text{(B-80)}$$

$$- h_2du - h_3dv + ydh_1 + udh_2 + vdh_3 =$$

$$= K_1dx + K_2dy + \frac{1}{\rho u} h_4 \sum_{i=1}^{n} \psi_i dx + \frac{1}{\rho u} \sum_{i=1}^{n} g_i \sigma_i \ dx \tag{B-81}$$

$$(vh_2 - uh_3)dv + \frac{1}{\rho} h_2 \ dP - h_4 \frac{a^2 u}{\rho} (\gamma-1) \ d\rho + yudh_1 - ua^2 dh_4 =$$

$$= \left[- h_4 a^2 \frac{v}{y} - a^2 K_3 + K_4\right] dx \tag{B-82}$$

$$udg_i = J_i dx - h_4 a^2 ua_i d\rho \qquad (i=1,..,n) \tag{B-83}$$

Along gas Mach lines,

$$\frac{dy}{dx} = \tan\ (\theta \pm \alpha) \tag{B-84}$$

$$a^2(vdu - udv) \pm \frac{1}{\rho} a^2 \cot\alpha \ dP = (udy - vdx) \left[a^2 \frac{v}{y} + \frac{1}{\rho} \sum_{i=1}^{n} \psi_i\right] \tag{B-85}$$

$$h_2du + h_3dv + \frac{1}{\rho} h_4 \ (dP - a^2 d\rho) + \sum_{i=1}^{n} g_i dC_i - ydh_1 \mp$$

$$\mp \tan\alpha \ (vdh_2 - udh_3) = \pm \tan\alpha \ (K_2dx - K_1dy) \pm$$

$$\pm \frac{1}{a^2} \tan\alpha \ (udy - vdx) \left[K_4 + \frac{1}{\rho} h_4 \sum_{i=1}^{n} \psi_i\right] \tag{B-86}$$

where θ is the flow angle and α is the Mach angle. In Eqs. (B-84), (B-85), and (B-86) the upper signs refer to left running Mach lines and the lower signs to right running Mach lines. Note that Eqs. (B-85) and (B-86) are actually two equations each when applied along the two Mach lines.

In summary, Eqs. (B-77) through (B-86) can be employed to evaluate the parameters x, y, u, v, P, ρ, C_i, h_1, h_2, h_3, h_4 and g_i throughout region ABC.

APPENDIX C

ANALYSIS OF VARIATION OF NOZZLE CONTOUR AND END POINT

In the consideration of variations of the nozzle contour $\eta(x)$ and nozzle end point X_c, only the line integral along AC in Eq. (18) contributes. The contour η enters this line integral in two ways, directly as a factor in the integrand, and as the value of the argument y of all gas properties. Thus,

$$u(x,y) = u[x,\eta(x)] \tag{C-1}$$

and similarly for the other properties. Variations in the gas properties holding x, y and η fixed were taken in Appendix B. In this Appendix, variations in the gas properties will be taken holding x fixed while variations are allowed in η. These variations are independent of those taken in Appendix B. Thus, along AC, the following variations in gas properties are allowable.

$$\delta u = \frac{\partial}{\partial \eta}\left\{u[x,\eta(x)]\right\}\delta\eta \qquad \text{for x fixed} \tag{C-2}$$

$$\delta u = u_y \delta\eta \tag{C-3}$$

In an analogous manner, one obtains

$$\delta v = v_y \delta\eta \tag{C-4}$$

$$\delta P = P_y \delta\eta \tag{C-5}$$

$$\delta\rho = \rho_y \delta\eta \tag{C-6}$$

Taking the variation of η along AC in Eq. (18) results in two effects. The first arises from variations in η under the integral sign, and the second results from the variation of the limits of integration. Since these effects are independent, they can be considered one at a time.

First, consider the variation of the limits of integration. At point A, no variations are allowed. Hence, no additional conditions are found. However, a variation in X_c, δX_c, is allowable. Noting that $(u\eta'-v) = 0$ along AC, the following result is obtained.

$$[(P-P_o)\eta\eta' + C_1 G(\eta,\eta',P)]_{X_c} \delta X_c = 0 \tag{C-7}$$

Since δX_c is arbitrary, the term in square brackets must equal zero. Therefore,

$$C_1 = - \frac{\eta_c \, \eta_c' \, (P_c - P_o)}{G(X_c)} \tag{C-8}$$

Next, consider the variation of η under the integral sign.

$$\int_A^C \left\{ \delta[(P-P_o)\eta\eta'] + C_1 \delta G(\eta,\eta',P) + C_2 \delta[\eta\rho(u\eta'-v)] \right\} dx = 0 \tag{C-9}$$

$$\int_A^C \Big\{ \eta\eta'\delta P + (P-P_o)\eta'\delta\eta + (P-P_o)\eta\delta\eta' + C_1 G_\eta \delta\eta + C_1 G_{\eta'} \delta\eta' +$$

$$+ C_1 G_p P_y \delta\eta + C_2(\eta\rho u)\delta\eta' + C_2[\eta'\delta(\eta\rho u) - \delta(\eta\rho v)] \Big\} dx = 0 \tag{C-10}$$

Substituting Eqs. (C-3) through (C-6) into Eq. (C-10) gives

$$\int_A^C \Big\{ [\eta\eta' P_y + (P-P_o)\eta' + C_1 G_\eta + C_1 G_p P_y + C_2\{\eta'(\eta\rho u)_y - (\eta\rho v)_y\}]\delta\eta \; +$$

$$+ [(P-P_o)\eta + C_1 G_{\eta'} + C_2(\eta\rho u)]\delta\eta' \Big\} dx = 0 \tag{C-11}$$

From the continuity equation, Eq. (1).

$$- (\eta\rho v)_y = (\eta\rho u)_x \tag{C-12}$$

Thus the fifth term under the integral in Eq. (C-11) can be written as

$$C_2 \{(\eta\rho u)_x + \eta'(\eta\rho u)_y\} \tag{C-13}$$

However, along AC,

$$\frac{d}{dx} = \frac{\partial}{\partial x} + \eta' \frac{\partial}{\partial y} \tag{C-14}$$

Equation (C-13) thus becomes

$$C_2 \frac{d}{dx} (\eta\rho u) \tag{C-15}$$

Integration by parts can be applied to the terms involving $\delta\eta'$ in Eq. (C-9). The following result, after introducing Eq. (C-15), is obtained.

$$\begin{aligned} &\left\{[(P-P_o)\eta + C_1 G_{\eta'} + C_2(\eta\rho u)]\ \delta\eta\right\} \Big|_{X_A}^{X_c} + \\ &+ \int_A^C \left\{[\eta\eta' P_y - \eta\frac{dP}{dx} + C_1 G_\eta + C_1 G_p P_y + C_2 \frac{d}{dx} (\eta\rho u) - \right. \\ &\qquad \left. - C_1 \frac{d}{dx} (G_{\eta'}) - \frac{d}{dx} (C_2 \eta\rho u)]\ \delta\eta\right\} dx = 0 \end{aligned} \tag{C-16}$$

In the terms arising from the limits of the integration by parts, the variation in $\delta\eta$ at X_A is zero since the flow must match the flow upstream of point A at point A. However, $\delta\eta$ at X_c is not fixed. Hence, the following result is obtained.

$$(P_c-P_o)\eta_c + C_1 G_{\eta'}(X_c) + C_2(X_c)\eta_c\rho_c u_c = 0 \tag{C-17}$$

Substituting Eq. (C-8) into Eq. (C-17) and solving for $C_2(X_c)$ gives

$$C_2(X_c) = -\frac{(P_c-P_o)}{\rho_c u_c}\left[1 - \frac{\eta_c' \, G_{\eta'}(X_c)}{G(X_c)}\right] \tag{C-18}$$

Returning to the line integral in Eq. (C-16), the following simplifications can be made.

$$-\frac{d}{dx}(C_2\eta\rho u) + C_2\frac{d}{dx}(\eta\rho u) = -\eta\rho u\frac{dC_2}{dx} \tag{C-19}$$

$$\eta\eta'\frac{\partial P}{\partial y} - \eta\frac{dP}{dx} = -\eta P_x \tag{C-20}$$

From the system momentum equations, Eqs. (2) and (3), P_x and P_y can be expressed as follows.

$$P_x = -\rho u(u_x + \frac{v}{u}u_y) = -\rho u\frac{du}{dx} \tag{C-21}$$

$$P_y = -\rho u(v_x + \frac{v}{u}v_y) = -\rho u\frac{dv}{dx} \tag{C-22}$$

Setting the coefficient of $\delta\eta$ in Eq. (C-16) equal to zero, and substituting Eqs. (C-19), (C-20), (C-21) and (C-22) into Eq. (C-16) gives the following result.

$$\frac{dC_2}{dx} = \frac{du}{dx} + \frac{(P_c-P_o)\eta_c\eta_c'}{G(X_c)}\,\frac{1}{\eta\rho u}\left[\frac{d}{dx}(G_{\eta'}) + \rho u G_p\frac{dv}{dx} - G_\eta\right] \tag{C-23}$$

Integrating Eq. (C-23) between the limits x and X_c, noting that the positive direction is from C to A, gives

$$C_2(x) = u - \frac{(P_c - P_o)\eta_c \eta_c'}{G(X_c)} \int_x^{X_c} \frac{1}{\eta\rho u} \left[\frac{d}{dx} (G_{\eta'}) + \rho u G_p \frac{dv}{dx} - G_\eta\right] dx + C_3 \qquad \text{(C-24)}$$

Evaluating Eq. (C-24) at point C and equating the result to the result found in Eq. (C-18) gives the following equation for C_3.

$$C_3 = - u_c - \frac{(P_c - P_o)}{\rho_c u_c} \left[1 - \frac{\eta_c' G_{\eta'}(X_c)}{G(X_c)}\right] \qquad \text{(C-25)}$$

Substituting Eq. (C-25) into Eq. (C-24) yields the final result for $C_2(x)$.

$$C_2(x) = (u - u_c) - \frac{(P_c - P_o)}{\rho_c u_c} \left[1 - \frac{\eta_c' G_{\eta'}(X_c)}{G(X_c)}\right] -$$

$$- \frac{(P_c - P_o)\eta_c \eta_c'}{G(X_c)} \int_x^{X_c} \frac{1}{\eta\rho u} \left[\frac{d}{dx} \left(\frac{\partial G}{\partial \eta'}\right) + \rho u \left(\frac{\partial G}{\partial P}\right) \frac{dv}{dx} - \left(\frac{\partial G}{\partial \eta}\right)\right] dx \qquad \text{(C-26)}$$

Thus, $C_2(x)$ can be determined along AC once the flow properties are known at point C.

In Appendix B, it was shown that along AC,

$$h_1\ [x, \eta(x)] = C_2(x) \qquad \text{(C-27)}$$

Hence, the Lagrange multiplier $h_1(x,y)$ can be evaluated along AC, giving a boundary condition for the determination of the Lagrange multipliers throughout the flow field.

APPENDIX D

METHOD OF CHARACTERISTICS

In many engineering problems the governing differential equations are systems of quasi-linear, non-homogeneous, partial differential equations of the first order for functions of two independent variables. A quasi-linear partial differential equation of the first order is defined as one that is non-linear in the dependent variables, but linear in the first partial derivatives of the dependent variables. Such a system of n equations can be written as*

$$L_i = a_{ij}\frac{\partial u^j}{\partial x} + b_{ij}\frac{\partial u^j}{\partial y} + c_i = 0 \qquad \begin{pmatrix} i = 1,\dots,n \\ j = 1,\dots,n \end{pmatrix} \tag{D-1}$$

where the superscript j identifies a particular dependent variable, and the coefficients a_{ij}, b_{ij}, and c_i depend on x, y, $u^1,\dots,u^j$. When expanded, this system of equations becomes

$$\left.\begin{array}{l}
L_1 = a_{11}u^1_x + a_{12}u^2_x+\dots+a_{1n}u^n_x + b_{11}u^1_y + b_{12}u^2_y+\dots+b_{1n}u^n_y + c_1 = 0 \\
L_2 = a_{21}u^1_x + a_{22}u^2_x+\dots+a_{2n}u^n_x + b_{21}u^1_y + b_{22}u^2_y+\dots+b_{2n}u^n_y + c_2 = 0 \\
\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\
\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\
\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\
L_n = a_{n1}u^1_x + a_{n2}u^2_x+\dots+a_{nn}u^n_x + b_{n1}u^1_y + b_{n2}u^2_y+\dots+b_{nn}u^n_y + c_n = 0
\end{array}\right\} \tag{D-2}$$

*In accordance with accepted convention, when an index is repeated, summation is carried out with respect to that index.

When such a system of equations is hyperbolic, the method of characteristics can be employed to obtain the desired solution. To simplify the presentation, the theory will first be developed for a system of two equations, and those results will then be extended to systems of n equations.

Consider a linear combination of the first order partial derivatives of a function $f(x,y)$.

$$af_x + bf_y + c = 0 \tag{D-3}$$

In Eq. (D-3), a, b, and c may be functions of f, x, and y. Equation (D-3) may be rearranged as follows

$$a(f_x + \frac{b}{a} f_y) + c = 0 \tag{D-4}$$

If $f(x,y)$ is restricted to be a continuous function having continuous derivatives, the following relationship must also be valid.

$$df = f_x dx + f_y dy \tag{D-5}$$

Equation (D-5) may be rewritten as follows

$$\frac{df}{dx} = (f_x + \frac{dy}{dx} f_y) \tag{D-6}$$

Comparing Eqs. (D-4) and (D-6), it is seen that Eq. (D-4) may be written as

$$a\ df + c\ dx = 0 \tag{D-7}$$

if the following relationship is forced to apply.

$$\frac{dy}{dx} = \frac{b}{a} \tag{D-8}$$

Equation (D-8) is the equation of a curve in the (x,y) plane if (b/a) is a real function. Such a curve, if it exists, is called a characteristic curve. Partial differential equations for which characteristic curves exist are termed hyperbolic equations. Along the characteristic curve, the function f(x,y) can be evaluated by applying Eq. (D-7), which is a total differential equation relating df to dx along the characteristic curve. An equation such as Eq. (D-7) is called a compatibility equation. Thus, the original partial differential equation specified by Eq. (D-3) can be replaced by the equivalent system of a characteristic curve along which a compatibility equation is valid. Such a replacement is the basis of the method of characteristics.

Consider now a system of two equations for the two dependent variables u(x,y) and v(x,y). Thus

$$\begin{aligned} L_1 &= a_{11}u_x + b_{11}u_y + a_{12}v_x + b_{12}v_y + c_1 = 0 \\ L_2 &= a_{21}u_x + b_{21}u_y + a_{22}v_x + b_{22}v_y + c_2 = 0 \end{aligned} \tag{D-9}$$

It is desired to find an equivalent system of characteristic curves and compatibility equations with which Eq. (D-9) can be replaced. Since both equations in Eq. (D-9) are coupled through the dependent variables u(x,y) and v(x,y), both equations must be considered simultaneously. This can be done by forming the differential operator

$$L = \sigma_1 L_1 + \sigma_2 L_2 \tag{D-10}$$

where σ_1 and σ_2 are arbitrary functions. Substituting Eq. (D-9) into Eq. (D-10) and putting the result into the form of Eq. (D-4) yields the following expression.

$$(a_{11}\sigma_1 + a_{21}\sigma_2)\left[u_x + \frac{(b_{11}\sigma_1 + b_{21}\sigma_2)}{(a_{11}\tau_1 + a_{21}\tau_2)} u_y\right] +$$

$$(a_{12}\sigma_1 + a_{22}\sigma_2)\left[v_x + \frac{(b_{12}\sigma_1 + b_{22}\sigma_2)}{(a_{12}\sigma_1 + a_{22}\sigma_2)} v_y\right] + (c_1\sigma_1 + c_2\sigma_2) = 0 \tag{D-11}$$

Equation (D-11) becomes

$$(a_{11}\sigma_1 + a_{21}\sigma_2)\, du + (a_{12}\sigma_1 + a_{22}\sigma_2)\, dv + (c_1\sigma_1 + c_2\sigma_2)\, dx = 0 \tag{D-12}$$

if the following equations are valid, where $\lambda = (dy/dx)$.

$$\lambda = \frac{b_{11}\sigma_1 + b_{21}\sigma_2}{a_{11}\sigma_1 + a_{21}\sigma_2} \tag{D-13}$$

$$\lambda = \frac{b_{12}\sigma_1 + b_{22}\sigma_2}{a_{12}\sigma_1 + a_{22}\sigma_2}$$

Equation (D-13) can be rearranged with σ_1 and σ_2 considered as the unknown variables.

$$\sigma_1(a_{11}\lambda - b_{11}) + \sigma_2(a_{21}\lambda - b_{21}) = 0 \tag{D-14}$$

$$\sigma_1(a_{12}\lambda - b_{12}) + \sigma_2(a_{22}\lambda - b_{22}) = 0$$

For Eq. (D-14) to have any solution for σ_1 and σ_2, other than the trivial solution $\sigma_1 = \sigma_2 = 0$, the determinant of the coefficients of σ_1 and σ_2 must be zero. Thus,

$$\begin{vmatrix} (a_{11}\lambda - b_{11}) & (a_{21}\lambda - b_{21}) \\ (a_{12}\lambda - b_{12}) & (a_{22}\lambda - b_{22}) \end{vmatrix} = 0 \qquad \text{(D-15)}$$

Expanding the determinant of Eq. (D-15) results in an equation of the following form for λ,

$$A\,\lambda^2 - 2B\,\lambda + C = 0. \qquad \text{(D-16)}$$

where

$$\begin{aligned} A &= (a_{11}a_{22} - a_{12}a_{21}) \\ B &= \tfrac{1}{2}(a_{11}b_{22} + a_{22}b_{11} - a_{12}b_{21} - a_{21}b_{12}) \qquad \text{(D-17)} \\ C &= (b_{11}b_{22} - b_{12}b_{21}) \end{aligned}$$

The terms A, B, and C are seen to be functions of the coefficients of the original system of partial differential equations, Eq. (D-9).

If $B^2 - AC < 0$, no real solutions for λ exist, and the characteristic curves are imaginary. Partial differential equations that result in imaginary characteristic curves are termed elliptic. If $B^2 - AC = 0$, one real characteristic direction exists through each point, and the system is called parabolic. If $B^2 - AC > 0$, two real characteristic directions exist through each point, and the system is called hyperbolic. The discussions which follow are concerned only with hyperbolic systems.

For hyperbolic systems, Eq. (D-1) has two distinct solutions λ_1 and λ_2. Hence, the two characteristic curves satisfy the two ordinary differential equations

$$\frac{dy}{dx} = \lambda_1 \quad \text{and} \quad \frac{dy}{dx} = \lambda_2 \tag{D-18}$$

Since the roots λ_1 and λ_2 are functions of x, y, u and v, the hyperbolic character of the system depends on the particular functions u(x,y) and v(x,y) under consideration. When a solution u(x,y) and v(x,y) is inserted into Eq. (D-18), the equations $dy/dx = \lambda_1(u,v,x,y)$ and $dy/dx = \lambda_2(u,v,x,y)$ are two ordinary differential equations of the first order that define two families of characteristic curves, or simply the characteristics, in the (x,y) plane.

Returning to Eq. (D-12), which is the general compatibility equation for the system, σ_1 and σ_2 can be eliminated in terms of λ from Eq. (D-13). Values of σ_1 and σ_2 from the solution of Eq. (D-14) can be introduced into Eq. (D-13) to solve either for σ_1 and σ_2 directly, or for one of σ's in terms of the other one. The results can be introduced into Eq. (D-12), thus eliminating both σ_1 and σ_2. The result is two compatibility equations (one for λ_1 and one for λ_2) relating du, dv, x and y along the characteristic curves given by Eq. (D-18). Thus, Eqs. (D-12) and (D-18) can replace the original system of partial differential equations, Eq. (D-9).

By analogy to the case of two partial differential equations discussed in the foregoing, the method of characteristics can be extended to a system of n partial differential equations. The governing equation for such a system is Eq. (D-1), repeated below.

$$L_i = a_{ij} \frac{\partial u^j}{\partial x} + b_{ij} \frac{\partial u^j}{\partial y} + c_i = 0 \qquad \begin{pmatrix} i = 1,\ldots,n \\ j = 1,\ldots,n \end{pmatrix} \tag{D-1}$$

The equations specified by Eq. (D-1) are combined in a linear manner to form the following differential operator.

$$L = \sigma_i\ L_i = \sigma_1\ L_1 + \sigma_2\ L_2 + \ldots + \sigma_n\ L_n = 0 \tag{D-19}$$

Putting Eq. (D-19) into the form of Eq. (D-4) results in the general compatibility equation for the system

$$(a_{ij}\sigma_i)\ du^j + c_i\sigma_i\ dx = 0 \qquad \begin{pmatrix} i = 1,\ldots,n \\ j = 1,\ldots,n \end{pmatrix} \tag{D-20}$$

In order for Eq. (D-20) to be valid, the following expression for λ must be true.

$$a_{ij}\sigma_i\lambda = b_{ij}\sigma_i \qquad \begin{pmatrix} i = 1,\ldots n \\ j = 1,\ldots,n \end{pmatrix} \tag{D-21}$$

Equation (D-21) consists of n equations for λ when j takes on values 1 through n. Solving for σ_i yields

$$\sigma_i(a_{ij}\lambda - b_{ij}) = 0 \qquad \begin{pmatrix} i = 1,\ldots,n \\ j = 1,\ldots,n \end{pmatrix} \tag{D-22}$$

For the solution of the system of equations defined by Eq. (D-22) to be other than zero, the determinant of the coefficients of σ_i must vanish:

$$|a_{ij}\lambda - b_{ij}| = 0 \qquad \begin{pmatrix} i = 1,\ldots,n \\ j = 1,\ldots,n \end{pmatrix} \tag{D-23}$$

The expanded determinant results in an algebraic equation of the nth degree for $\lambda = dy/dx$, giving n roots, λ_m (m = 1, 2,....,n), which determine n characteristic directions. If all n roots are distinct and real, the system is totally hyperbolic. In that case there are n families of characteristics satisfying the ordinary differential equations.

$$\frac{dy}{dx} = \lambda_m \qquad (m = 1, \ldots, n) \qquad \text{(D-24)}$$

Once the λ_m are determined from Eq. (D-24), the σ_i can be evaluated from Eq. (D-21). In general, all the σ_i but one can be solved for in terms of the remaining one which can then be cancelled out in Eq. (D-20). These results, when substituted in the general compatibility equation, Eq. (D-20), determine the compatibility equations for the system. Equations (D-20) and (D-24) can replace the original system of partial differential equations, Eq. (D-1).

The initial value problem can now be formulated for the above system of hyperbolic differential equations. Assume a curve Γ_o is given in the (x,y) plane, and continuous values of u^j are arbitrarily prescribed along Γ_o as illustrated in Fig. (D-1). The problem is to determine, in the neighborhood of Γ_o, a solution u^j of the system that has the prescribed initial values along Γ_o. By replacing the original system of partial differential equations by the characteristic system, the problem reduces to solving the total differential equations given by the compatibility equations along the characteristic curves. In general, these equations are non-linear and coupled. For that reason, a solution procedure based on a numerical iteration technique is required. The compatibility equations,

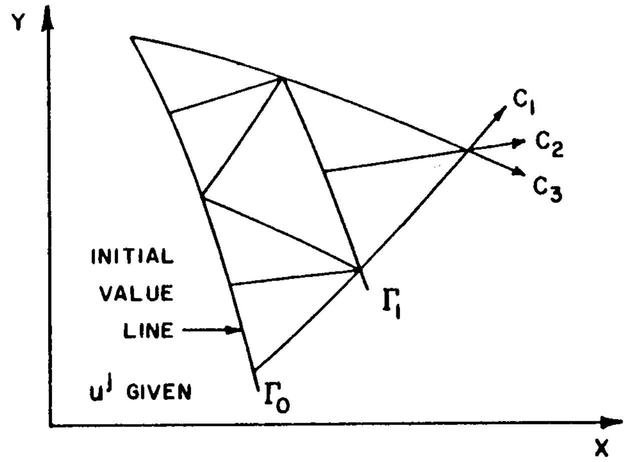

FIGURE D-1. CHARACTERISTIC INITIAL VALUE LINE AND SOLUTION NET

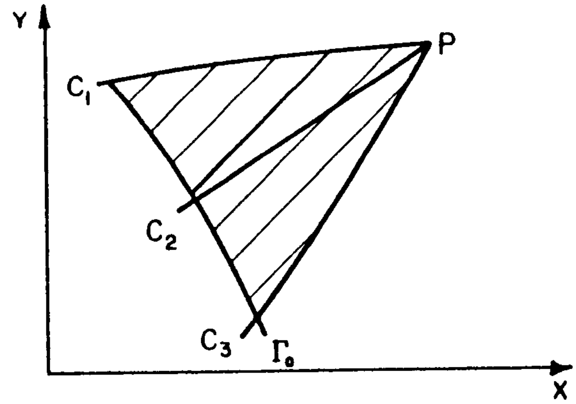

FIGURE D-2. DOMAIN OF DEPENDENCE

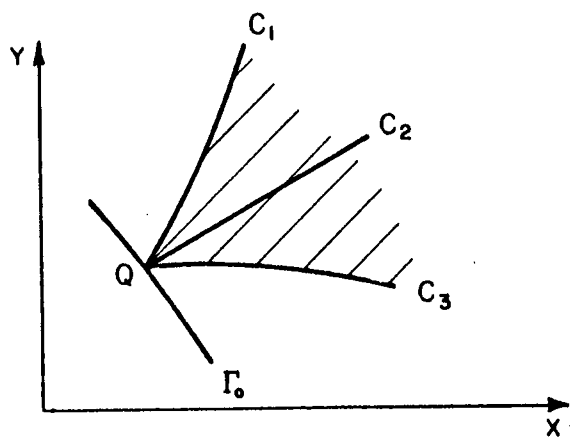

FIGURE D-3. RANGE OF INFLUENCE

each of which is valid along one or more of the characteristic curves, can be written in finite difference form, as can the equations of the characteristic curves. By moving along the characteristic curves, the initial values of u^j along Γ_o can be extended into the domain enclosed by the outermost characteristic curves passing through the initial data curve Γ_o. By continuing in small steps along Γ_o, a new curve, Γ_1, can be obtained with all the values of u^j determined along that curve, as illustrated in Fig. D-1.

The foregoing considerations result in the concepts of domain of dependence and range of influence. Figure D-2 illustrates the domain of dependence of a point P, which is the region in the (x,y) plane bounded by the outermost characteristics passing through the initial value line Γ_o, and is the region wherein the solution of the initial value problem can be established. Figure D-3 illustrates the range of influence of a point Q on the initial value line Γ_o, which is the region in the (x,y) plane containing all of the points which are influenced by the initial data at point Q. The range of influence is comprised of all of the points having a domain of dependence containing the point Q. Therefore, it is the region between the two outermost characteristics passing through point Q.

For a solution to be possible, the initial value line cannot be characteristic at any place unless initial data are given along two intersecting characteristic curves. Several types of domains having different types of initial value lines can be solved.

By applying the method of characteristics as summarized in the foregoing discussion, it is possible to solve many complicated systems of partial differential equations, provided the system is quasi-linear and hyperbolic. The latter conditions are frequently encountered in fluid flow problems.

APPENDIX E

CHARACTERISTICS RESULTING FROM VARIATIONS OF GAS PROPERTIES

In this section, the method of characteristics as developed in Appendix D will be employed to obtain the characteristic and compatibility equations for the system of partial differential equations resulting from the variations of gas properties. It is shown that the characteristic curves are the Mach lines and the gas streamline, and that there are a sufficient number of compatibility equations valid on these characteristic curves with which to replace the original system of partial differential equations.

The system of equations to be considered consists of the ten partial differential equations, Eqs. (1) through (5), (B-65), (B-67), (B-69), (B-73), and (B-75), which govern the variables u, v, P, ρ, C_i, h_1, h_2, h_3, h_4, and g_i. These equations are repeated below for convenience.

$$\rho u_x + \rho v_y + u\rho_x + u\rho_y = -\frac{\rho v}{y} \tag{E-1}$$

$$\rho(uu_x + vu_y) + P_x = 0 \tag{E-2}$$

$$\rho(uv_x + vv_y) + P_y = 0 \tag{E-3}$$

$$uP_x + vP_y - a^2(u\rho_x + v\rho_y) = \sum_{i=1}^{n} \psi_i \tag{E-4}$$

$$\rho u(C_i)_x + \rho v(C_i)_y = \sigma_i \qquad (i=1,..,n) \tag{E-5}$$

$$- h_2 u_x - h_3 v_x - \frac{1}{\rho} h_4 (P_x - a^2 \rho_x) - \sum_{i=1}^{n} g_i (C_i)_x +$$

$$+ y(h_1)_x + u(h_2)_x + v(h_2)_y = K_1 \tag{E-6}$$

$$- h_2 u_y - h_3 v_y - \frac{1}{\rho} h_4 (P_y - a^2 \rho_y) - \sum_{i=1}^{n} g_i (C_i)_y +$$

$$+ y(h_1)_y + u(h_3)_x + v(h_3)_y = K_2 \tag{E-7}$$

$$h_4 u_x + h_4 v_y + h_4 \frac{1}{P} a^2 (u\rho_x + v\rho_y) + (h_2)_x + (h_3)_y +$$

$$+ u(h_4)_x + v(h_4)_y = K_3 \tag{E-8}$$

$$\frac{1}{\rho} h_2 P_x + \frac{1}{\rho} h_3 P_y + yu(h_1)_x + yv(h_1)_y + a^2 (h_2)_x + a^2 (h_3)_y = K_4 \tag{E-9}$$

$$h_4 a^2 a_i (u\rho_x + v\rho_y) + \rho u(g_i)_x + \rho v(g_i)_y = J_i \qquad (i=1,..,n) \tag{E-10}$$

The non-homogeneous terms K_1, K_2, K_3, K_4 and J_i are defined by Eqs. (B-66), (B-68), (B-70), (B-74), and (B-76). These terms involve the gas properties u, v. P, ρ, and C_i, and the Lagrange multipliers h_1, h_2, h_3, h_4, and g_i.

As shown in Appendix D, the characteristic curves are found by expanding the following determinant.

$$|a_{ij}\lambda - b_{ij}| = 0 \tag{E-11}$$

The detailed form of Eq. (E-11) is shown below.

$$\left|\begin{array}{c|c} \text{[Gas]} & \text{Zeros} \\ \hline \begin{array}{c}\text{Terms Coupling}\\ \text{Multipliers to}\\ \text{Gas Properties}\end{array} & \text{[Multipliers]} \end{array}\right| = 0 \qquad \text{(E-12)}$$

$$[\text{Gas}] = \left|\begin{array}{ccccccccc} \rho\lambda & -\rho & 0 & (u\lambda-v) & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ \rho(u\lambda-v) & 0 & \lambda & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ 0 & \rho(u\lambda-v) & -1 & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ 0 & 0 & (u\lambda-v) & -a^2(u\lambda-v) & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ 0 & 0 & 0 & 0 & \rho(u\lambda-v)_1 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ 0 & 0 & 0 & 0 & 0 & \cdot\cdot & \rho(u\lambda-v)_i & \cdot\cdot & 0 \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ 0 & 0 & 0 & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & \rho(u\lambda-v)_n \end{array}\right| \qquad \text{(E-13)}$$

The terms denoted by $\rho(u\lambda-v)_i$ arise from the coefficients of Eq. (E-5), the species continuity equation. As indicated, there are n columns and rows in Eq. (E-13) corresponding to the n chemical species being considered, in addition to the four columns and rows corresponding to Eqs. (E-1) through (E-4). The rows and columns of double dots •• indicate the position of the additional terms when applicable.

$$[\text{Multipliers}] = \begin{vmatrix} y\lambda & (u\lambda-v) & 0 & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ -y & 0 & (u\lambda-v) & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ 0 & \lambda & -1 & (u\lambda-v) & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ y(u\lambda-v) & a^2\lambda & -a^2 & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ 0 & 0 & 0 & 0 & \rho(u\lambda-v)_1 & \cdot\cdot & 0 & \cdot\cdot & 0 \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ 0 & 0 & 0 & 0 & 0 & \cdot\cdot & \rho(u\lambda-v)_i & \cdot\cdot & 0 \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ 0 & 0 & 0 & 0 & 0 & \cdot\cdot & 0 & \cdot\cdot & \rho(u\lambda-v)_n \end{vmatrix} \qquad \text{(E-14)}$$

As in Eq. (E-13), the terms $\rho(u\lambda-v)_i$ arise from the coefficients of the n equations contained in Eq. (E-10).

Since the upper right corner of the determinant given in Eq. (E-12) is filled with zeros, the expansion of Eq. (E-12) reduces to the following form.

$$|[\text{Gas}]| \times |[\text{Multipliers}]| = 0 \qquad \text{(E-15)}$$

Setting Eq. (E-13) equal to zero results in the following expression.

$$[\lambda^2(u^2 - a^2) - 2uv\lambda + (v^2 - a^2)]\ (u\lambda - v)^{2+n} = 0 \qquad \text{(E-16)}$$

The characteristic curves are found by solving for λ, thus giving for this system the Mach lines each appearing once and the gas streamline appearing

(2+n) times.

$$\lambda = \frac{dy}{dx} = \frac{v}{u} \tag{E-17}$$

$$\lambda = \frac{dy}{dx} = \frac{uv \pm a^2\sqrt{M^2 - 1}}{u^2 - a^2} \tag{E-18}$$

The flow angle and the Mach angle are defined by the following equations.

$$\theta = \tan^{-1} \frac{v}{u} \tag{E-19}$$

$$\alpha = \sin^{-1} \frac{1}{M} \tag{E-20}$$

In terms of θ and α, Eq. (E-18) becomes

$$\lambda = \frac{dy}{dx} = \tan(\theta \pm \alpha) \tag{E-21}$$

Setting Eq. (E-14) equal to zero gives the following result.

$$[\lambda^2(u^2 - a^2) - 2uv\lambda + (v^2 - a^2)]\ (u\lambda - v)^{2+n} = 0 \tag{E-22}$$

Equation (E-22) is the same as Eq (E-16). Hence, the characteristic curves obtained from Eq. (E-22) will again be the Mach lines and the gas streamline appearing (2+n) times.

Thus, the characteristic curves obtained for the system of partial differential equations, Eqs. (E-1) through (E-10), are the gas streamline appearing (4+2n) times, and the gas Mach lines each appearing two times.

A total of (8+2n) distinct, real characteristic curves thus exist, making the system totally hyperbolic.

To determine the compatibility equations for the system of partial differential equations, Eqs. (E-1) through (E-10), the method developed in Appendix D will be employed. The general compatibility equation is found by forming the sum $\sigma_i L_i$, where the σ_i are unknown functions. In the present case, Eqs. (E-1) through (E-4) will be multiplied by σ_1 through σ_4, Eqs. (E-6) through (E-9) will be multiplied by σ_5 through σ_8, and Eqs. (E-5) and (E-10) will be multiplied by θ_i and η_i respectively. These σ's, θ's, and η's are arbitrary functions employed in the determination of the compatibility equations, and are not the same as the σ's, θ's, and η's defined in the Nomenclature, Section V. Thus after some grouping, the following equation is obtained.

$$\begin{aligned}
&(\rho\sigma_1 + \rho u\sigma_2 - h_2\sigma_5 + h_4\sigma_7)du + (\rho u\sigma_3 - h_3\sigma_5)dv + \\
&+ (\sigma_2 + u\sigma_4 - \frac{1}{\rho} h_4\sigma_5 + \frac{1}{\rho} h_2\sigma_8)dP + \Big[u\sigma_1 - a^2u\sigma_4 + \frac{1}{\rho} h_4a^2\sigma_5 + \\
&+ \frac{1}{P} h_4a^2u\sigma_7 + h_4a^2u \sum_{i=1}^{n} \eta_i a_i\Big]d\rho + \sum_{i=1}^{n} (\rho u\theta_i - \sigma_5 g_i)dC_i + \\
&+ (y\sigma_5 + yu\sigma_8)dh_1 + (u\sigma_5 + \sigma_7 + a^2\sigma_8)dh_2 + (u\sigma_6)dh_3 + \\
&+ (u\sigma_7)dh_4 + \sum_{i=1}^{n} \rho u\eta_i dg_i = \sum_{j=1}^{8} \sigma_j N_j dx + \sum_{i=1}^{n} (\theta_i\sigma_i + \eta_i J_i)dx
\end{aligned} \qquad \text{(E-23)}$$

In Eq. (E-23), N_j represents the non-homogeneous terms in Eqs. (E-1) through

(E-4) and (E-6) through (E-9). The terms σ_i and J_i are the non-homogeneous terms arising in Eqs. (E-5) and (E-10) respectively.

The equations for λ, obtained as discussed in Appendix D, are as follows.

$$\lambda = \frac{\rho v\sigma_2 - h_2\sigma_6}{\rho v_1 + \rho u\sigma_2 - h_2\sigma_5 + h_4\sigma_7} \tag{E-24}$$

$$\lambda = \frac{\rho\sigma_1 + \rho v\sigma_3 - h_3\sigma_6 + h_4\sigma_7}{\rho u\sigma_3 - h_3\sigma_5} \tag{E-25}$$

$$\lambda = \frac{\sigma_3 + v\sigma_4 - \frac{1}{\rho} h_4\sigma_6 + \frac{1}{\rho} h_3\sigma_8}{\sigma_2 + u\sigma_4 - \frac{1}{\rho} h_4\sigma_5 + \frac{1}{\rho} h_2\sigma_8} \tag{E-26}$$

$$\lambda = \frac{v\sigma_1 - a^2 v\sigma_4 + \frac{1}{\rho} h_4 a^2\sigma_6 + \frac{1}{P} h_4 a^2 v\sigma_7 + h_4 a^2 v \sum_{i=1}^{n} \eta_i a_i}{u\sigma_1 - a^2 u\sigma_4 + \frac{1}{\rho} h_4 a^2\sigma_5 + \frac{1}{P} h_4 a^2 u\sigma_7 + h_4 a^2 u \sum_{i=1}^{n} \eta_i a_i} \tag{E-27}$$

$$\lambda = \frac{\rho v\theta_i - \sigma_6 g_i}{\rho u\theta_i - \sigma_5 g_i} \qquad (i=1,..,n) \tag{E-28}$$

$$\lambda = \frac{y\sigma_6 + yv\sigma_8}{y\sigma_5 + yu\sigma_8} \tag{E-29}$$

$$\lambda = \frac{v\sigma_5}{u\sigma_5 + \sigma_7 + a^2\sigma_8} \tag{E-30}$$

$$\lambda = \frac{v\sigma_6 + \sigma_7 + a^2\sigma_8}{u\sigma_6} \tag{E-31}$$

$$\lambda = \frac{v\sigma_7}{u\sigma_7} \tag{E-32}$$

$$\lambda = \frac{\rho v \eta_i}{\rho u \eta_i} \qquad (i=1,..,n) \tag{E-33}$$

Rearranging Eqs. (E-24) through (E-33) gives the following equations for σ_1 through σ_8, θ_i, and η_i, in terms of the characteristic direction λ.

$$\sigma_1(\rho\lambda) + \sigma_2\rho(u\lambda-v) + \sigma_5(-h_2\lambda) + \sigma_6(h_2) + \sigma_7(h_4\lambda) = 0 \tag{E-34}$$

$$\sigma_1(-\rho) + \sigma_3\rho(u\lambda-v) + \sigma_5(-h_3\lambda) + \sigma_6(h_3) + \sigma_7(-h_4\lambda) = 0 \tag{E-35}$$

$$\sigma_2(\lambda) + \sigma_3(-1) + \sigma_4(u\lambda-v) + \sigma_5(-\frac{1}{\rho} h_4\lambda) + \sigma_6(\frac{1}{\rho} h_4) + \\ + \sigma_8 \frac{1}{\rho}(h_2\lambda - h_3) = 0 \tag{E-36}$$

$$\sigma_1(u\lambda-v) + \sigma_4 a^2(v-u\lambda) + \sigma_5(\frac{1}{\rho} h_4 a^2\lambda) + \sigma_6(-\frac{1}{\rho} h_4 a^2) + \\ + \sigma_7(\frac{1}{p} h_4 a^2)(u\lambda-v) + h_4 a^2(u\lambda-v) \sum_{i=1}^{n} \eta_i a_i = 0 \tag{E-37}$$

$$\rho(u\lambda-v)\theta_i + \sigma_5(-g_i\lambda) + \sigma_6(g_i) = 0 \qquad (i=1,..,n) \tag{E-38}$$

$$\sigma_5(\lambda) + \sigma_6(-1) + \sigma_8(u\lambda-v) = 0 \tag{E-39}$$

$$\sigma_5(u\lambda-v) + \sigma_7(\lambda) + \sigma_8(a^2\lambda) = 0 \tag{E-40}$$

$$\sigma_6(u\lambda-v) + \sigma_7(-1) + \sigma_8(-a^2) = 0 \tag{E-41}$$

$$\sigma_7(u\lambda-v) = 0 \tag{E-42}$$

$$\rho(u\lambda - v)\eta_i = 0 \qquad (i=1,..,n) \qquad \text{(E-43)}$$

Equations (E-34) through (E-43) may now be solved for σ_1 through σ_8, θ_i, and η_i, for each specific value of λ. The results may be substituted back into the general compatibility equation, Eq. (E-23), to obtain the particular compatibility equation which is valid on the characteristic curve pertinent to the value of λ chosen. In the present case, only two separate equations for λ exist, Eqs. (E-17) and (E-18). Even though Eq. (E-18) is actually two equations when the plus and minus signs are considered, the combined form of the equation may be employed to obtain a set of compatibility equations which will then be valid on both characteristics obtained from Eq. (E-18). The compatibility equations valid on the gas streamline will be determined first.

On the gas streamline, Eq. (E-17) becomes

$$(u\lambda - v) = 0 \qquad \text{(E-44)}$$

Substituting Eq. (E-44) into Eqs. (E-34) through (E-43) and solving the resulting system of equations gives the following results.

$$\sigma_1 = \frac{1}{\rho} h_4 a^2 \sigma_8 \qquad \text{(E-45)}$$

$$\sigma_1 = \frac{1}{\rho} h_4 a^2 \sigma_8 \qquad \text{(E-46)}$$

$$\sigma_3 = \lambda\sigma_2 + \frac{1}{\rho} (h_2\lambda - h_3)\sigma_8 \qquad \text{(E-47)}$$

$$\sigma_6 = \lambda\sigma_5 \qquad \text{(E-48)}$$

$$\sigma_6 = \lambda\sigma_5 \qquad (i=1,..,n) \qquad \text{(E-49)}$$

$$\sigma_6 = \lambda\sigma_5 \qquad \text{(E-50)}$$

$$\sigma_7 = -a^2\sigma_8 \qquad \text{(E-51)}$$

$$\sigma_7 = -a^2\sigma_8 \qquad \text{(E-52)}$$

$$\sigma_7(0) = 0 \qquad \text{(E-53)}$$

$$\eta_i(0) = 0 \qquad (i=1,..,n) \qquad \text{(E-54)}$$

Of the above ten equations, four independent relationships are given by Eqs. (E-45), (E-47), (E-48) and (E-51). Observe that θ_i and η_i are arbitrary. Thus, four equations exist relating the eight σ_i's. Note that σ_4 does not appear in the system of equations, and is therefore arbitrary. Hence, three of the remaining seven σ_i's are arbitrary and independent. If σ_2, σ_4, σ_5, and σ_8 are chosen as being arbitrary, σ_1, σ_3, σ_6, and σ_7 can be expressed in terms of these four by the four equations obtained above. Substituting those four equations into the general compatibility equation, Eq. (E-23), and solving for the coefficients of the four arbitrary σ_i's, the arbitrary θ_i's, and the arbitrary η_i's, gives the following result.

$$\sigma_2 \{\rho u du + \rho v dv + dP\} + \sigma_4 \{u dP - a^2 u d\rho - \sum_{i=1}^{n} \psi_i dx\} +$$

$$+ \sigma_5 \{-h_2 du - h_3 dv - \frac{1}{\rho} h_4 (dP - a^2 d\rho) - \sum_{i=1}^{n} g_i dC_i +$$

$$+ y dh_1 + u dh_2 + v dh_3 - (K_1 dx + K_2 dy)\} +$$

$$+ \sigma_8 \{h_4 a^2 du - h_4 a^2 du + u(h_2\lambda - h_3) dv + \frac{1}{\rho} h_2 dP +$$

$$+ \frac{1}{\rho} h_4 a^2 u d\rho - a^2 \frac{1}{P} h_4 a^2 u d\rho + y u dh_1 - a^2 dh_2 + a^2 dh_2 -$$

$$- a^2 u dh_4 + a^2 K_3 dx - K_4 dx + \frac{1}{y} h_4 a^2 v dx\} +$$

$$+ \sum_{i=1}^{n} \theta_i \{\rho u dC_i - \sigma_i dx\} +$$

$$+ \sum_{i=1}^{n} \eta_i \{h_4 a^2 a_i u d\rho + \rho u dg_i - J_i dx\} = 0 \qquad \text{(E-55)}$$

Equation (E-17) has been substituted into Eq. (E-55) to eliminate λ wherever it appeared. Since σ_2, σ_4, σ_5, σ_8, θ_i, and η_i are all arbitrary, their coefficients must be identically zero. Thus the following compatibility equations valid on a gas streamline are obtained.

$$\rho u du + \rho v dv + dP = 0 \qquad \text{(E-56)}$$

$$dP - a^2 d\rho = \frac{1}{u} \sum_{i=1}^{n} \psi_i dx \qquad \text{(E-57)}$$

$$\rho u dC_i = \sigma_i dx \qquad (i=1,\ldots,n) \tag{E-58}$$

$$- h_2 du - h_3 dv - \frac{1}{\rho} h_4 \ (dP - a^2 d\rho) - \sum_{i=1}^{n} g_i dC_i + y dh_1 +$$

$$+ u dh_2 + v dh_3 = K_1 dx + K_2 dy \tag{E-59}$$

$$(vh_2 - uh_3) dv + \frac{1}{\rho} h_2 \ dP - \frac{1}{\rho} h_4 a^2 u \ (\gamma-1) d\rho + yu dh_1 -$$

$$- ua^2 dh_4 = - \frac{1}{y} h_4 a^2 v \ dx - a^2 K_3 dx + K_4 dx \tag{E-60}$$

$$\rho u dg_i = J_i dx - h_4 a^2 a_i u d\rho \qquad (i=1,\ldots,n) \tag{E-61}$$

On Mach lines, Eq. (E-18) becomes

$$\lambda^2 (u^2 - a^2) - 2uv\lambda + (v^2 - a^2) = 0 \tag{E-62}$$

Proceeding as before by substituting Eq. (E-62) into Eqs. (E-34) through (E-43), the following equations are obtained.

$$\sigma_2 = - \frac{\lambda a^2}{(u\lambda - v)} \sigma_4 - \frac{1}{\rho} \left[h_2 + \frac{\lambda a^2}{(u\lambda - v)} h_4 \right] \sigma_8 \tag{E-63}$$

$$\sigma_3 = \frac{\lambda a^2}{(u\lambda - v)} \sigma_4 + \frac{1}{\rho} \left[\frac{a^2}{(u\lambda - v)} h_4 - h_3 \right] \sigma_8 \tag{E-64}$$

$$\sigma_2 \lambda - \sigma_3 + \sigma_4 (u\lambda - v) + \frac{1}{\rho} \left[(u\lambda - v) h_4 + (h_2 \lambda - h_3) \sigma_8 \right] = 0 \tag{E-65}$$

$$\sigma_1 = a^2 \sigma_4 + \frac{1}{\rho} h_4 a^2 \sigma_8 \tag{E-66}$$

$$\theta_i = -\frac{1}{\rho} h_4 a^2 a_i \sigma_8 - \frac{1}{\rho} g_i \sigma_8 \qquad (i=1,..,n) \tag{E-67}$$

$$\sigma_8(0) = 0 \tag{E-68}$$

$$\sigma_5 = -\frac{a^2\lambda}{(u\lambda - v)} \sigma_8 \tag{E-69}$$

$$\sigma_6 = \frac{a^2}{(u\lambda - v)} \sigma_8 \tag{E-70}$$

$$\sigma_7 = 0 \tag{E-71}$$

$$\eta_i = 0 \qquad (i=1,..,n) \tag{E-72}$$

Multiplying Eq. (E-63) by $-\lambda$ and adding the result to Eq. (E-64) gives Eq. (E-65). Hence, Eq. (E-65) is not an independent equation. The eight equations, Eqs. (E-63), (E-64), (E-66), (E-67), and (E-69) through (E-72), relate the σ_i's, θ_i's, and η_i's. Thus, two of the σ_i's are arbitrary. Choosing σ_4 and σ_8 to be arbitrary, substituting the above equations into the general compatibility equation, Eq. (E-23), setting the coefficients of σ_4 and σ_8 equal to zero, and simplifying the result gives the following two equations.

$$a^2(vdu - udv) \pm \frac{1}{\rho} a^2 \cot\alpha \, dP = (udy - vdx) \left[\frac{a^2 v}{y} + \frac{1}{\rho} \sum_{i=1}^{n} \psi_i\right] \tag{E-73}$$

$$h_2du + h_3dv + \frac{1}{\rho} h_4 (dP - a^2d\rho) + \sum_{i=1}^{n} g_i dC_i - ydh_1 \mp$$

$$\mp \tan\alpha(vdh_2 - udh_3) = \pm \tan\alpha(K_2dx - K_1dy) \pm$$

$$\frac{\pm \tan\alpha(udy - vdx)}{a^2} \left[K_4 + \frac{1}{\rho} h_4 \sum_{i=1}^{n} \psi_i\right] \tag{E-74}$$

The upper signs in Eqs. (E-73) and (E-74) pertain to left running Mach lines and the lower signs to right running Mach lines. Equations (E-73) and (E-74) are each valid on both Mach lines, thus giving four independent equations.

In summary, for the system of equations (E-1) through (E-10), (8+2n) characteristic equations were found of which three, the two Mach lines and the gas streamline, are distinct. A total of (8+2n) compatibility equations, each valid along one of the characteristic curves, were found. Thus the original system of partial differential equations may be replaced by the system of characteristic and compatibility equations developed in this Appendix. Figure E-1 illustrates the characteristic net for the present system, indicating which compatibility equations are valid on which characteristic curves.

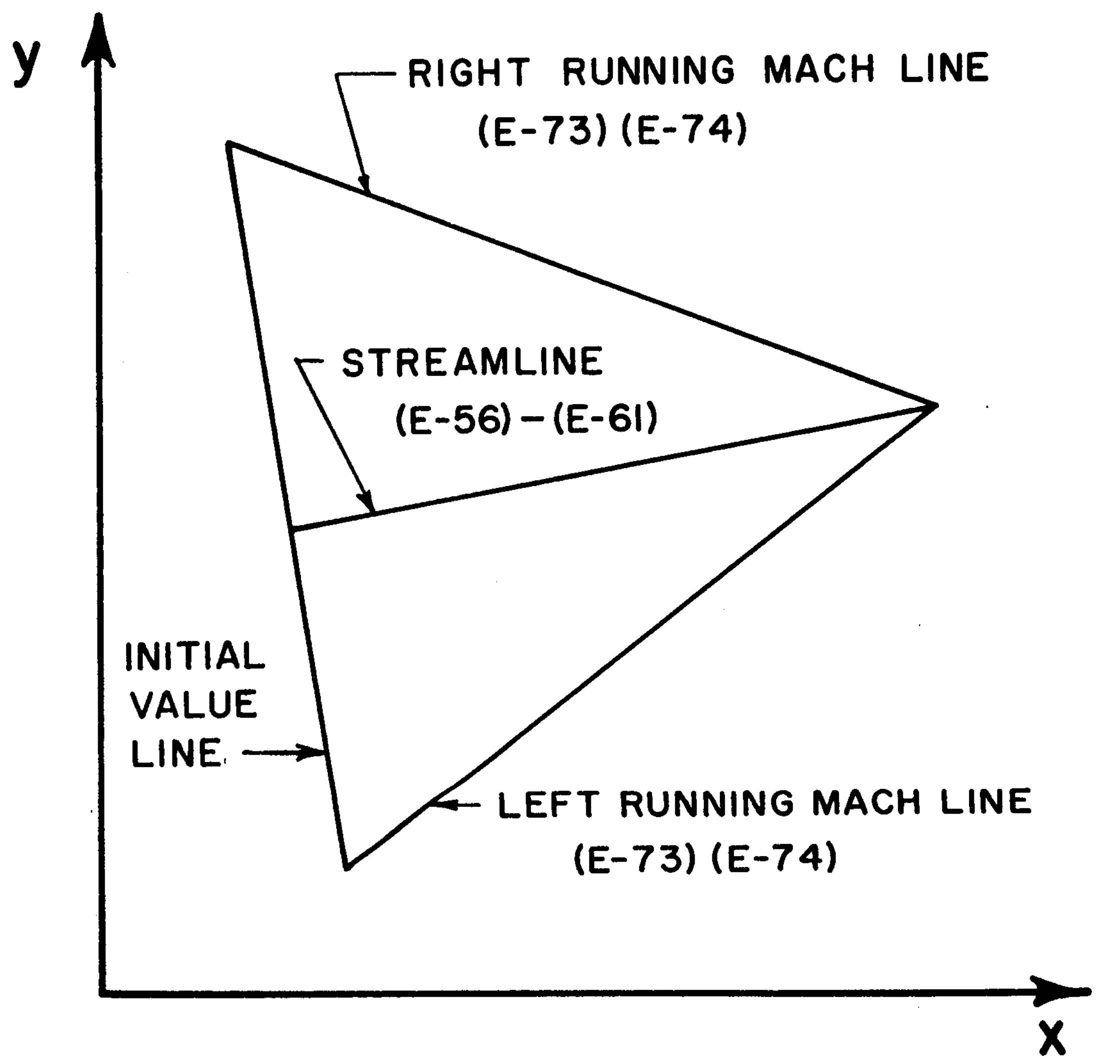

FIGURE E-1. CHARACTERISTIC NETWORK FOR GAS PROPERTIES AND LAGRANGE MULTIPLIERS

APPENDIX F

EVALUATION OF DERIVATIVES OF THERMODYNAMIC FUNCTIONS

The set of partial differential equations, Eqs. (35) through (39), obtained for determining the Lagrange multipliers in region ABC contains some complicated derivatives of the functions ψ_i and σ_i. These derivatives appear in the terms K_3, K_4, and J_i defined by Eqs. (42), (43), and (44) respectively. These terms are repeated below for convenience of discussion.

$$K_3 = -h_4 \sum_{i=1}^{n} \psi_{iP} - \sum_{i=1}^{n} g_i \sigma_{iP} \tag{F-1}$$

$$K_4 = h_4 \frac{a^2}{P} \sum_{i=1}^{n} \psi_i - h_4 \sum_{i=1}^{n} (a^2 \psi_{iP} + \psi_{i\rho}) - \sum_{i=1}^{n} g_i (a^2 \sigma_{iP} + \sigma_{i\rho}) + \frac{1}{\rho} \sum_{i=1}^{n} (h_4 a^2 a_i + g_i) \sigma_i \tag{F-2}$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} (\psi_k)_{C_i} - \sum_{k=1}^{n} g_k (\sigma_k)_{C_i} \qquad (i=1,\ldots,n) \tag{F-3}$$

In this Appendix, these terms are expressed in terms of the fundamental thermodynamic properties of the system.

The functions ψ_i and σ_i as defined by Eqs. (7) and (6) respectively both depend on the temperature T in addition to the pressure P, density ρ, and species mass fractions C_k. In the optimization analysis, these parameters were assumed to depend only on P, ρ, and C_k, the temperature dependence being eliminated by substitution of the perfect gas law, Eq. (8).

This transformation is accomplished here by employing two different functional forms for ψ_i and σ_i. From Eq. (7),

$$\sum_{i=1}^{n} \psi_i'(\rho,T,C_k) = \sum_{i=1}^{n} \phi_i'(T,C_k)\sigma_i'(\rho,T,C_k) \tag{F-4}$$

where

$$\phi_i'(T,C_k) = [\gamma R_i T - (\gamma-1)h_i] \tag{F-5}$$

The function ψ_i and ψ_i' are equal for compatable values of the arguments of each functional form.

$$\psi_i(P,\rho,C_k) = \psi_i'(\rho,T,C_k) \tag{F-6}$$

Taking derivatives of Eq. (F-6) gives

$$\psi_{iP} = \psi_{iP}' + \psi_{iT}' T_P = \psi_{iT}' T_P \tag{F-7}$$

$$\psi_{i\rho} = \psi_{i\rho}' + \psi_{iT}' T_\rho \tag{F-8}$$

$$(\psi_k)_{C_i} = (\psi_k')_{C_i} + \psi_{kT}' T_{C_i} \tag{F-9}$$

Substituting Eq. (F-4) into Eqs. (F-7) through (F-9) gives the following results.

$$\psi_{iP} = (\phi_{iT}' \sigma_i' + \phi_i' \sigma_{iT}')T_P \tag{F-10}$$

$$\psi_{i\rho} = \phi_i' \, \sigma_{i\rho}' + (\phi_{iT}' \, \sigma_i' + \phi_i' \, \sigma_{iT}') T_\rho \tag{F-11}$$

$$(\psi_k)_{C_i} = (\phi_k')_{C_i} \, \sigma_k' + \phi_k' \, (\sigma_k')_{C_i} + (\phi_{kT}' \, \sigma_k' + \phi_k' \, \sigma_{kT}') T_{C_i} \tag{F-12}$$

The species source function σ_i can be treated in a similar manner. Thus,

$$\sigma_i(P,\rho,C_k) = \sigma_i'(\rho,T,C_k) \tag{F-13}$$

where σ_i' is given by the law of mass action in Eq. (6).

$$\sigma_i' = W_i \sum_{r=1}^{N} (\nu_{ir}'' - \nu_{ir}') \left[K_{fr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu_{jr}'} - K_{rr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu_{jr}''} \right] \tag{F-14}$$

The specific reaction rate constants K_{fr} and K_{rr} are functions of temperature only. Taking derivatives of Eq. (F-13) gives

$$\sigma_{iP} = \sigma_{iP}' + \sigma_{iT}' \, T_P = \sigma_{iT}' \, T_P \tag{F-15}$$

$$\sigma_{i\rho} = \sigma_{i\rho}' + \sigma_{iT}' \, T_\rho \tag{F-16}$$

$$(\sigma_k)_{C_i} = (\sigma_k')_{C_i} + \sigma_{kT}' \, T_{C_i} \tag{F-17}$$

The perfect gas law is given by Eq. (8).

$$T = \frac{P}{\rho \sum_{k=1}^{n} C_k R_k} \tag{F-18}$$

Taking partial derivatives of Eq. (F-18) results in the following expressions.

$$T_P = \frac{T}{P} \tag{F-19}$$

$$T_\rho = \frac{T}{\rho} \tag{F-20}$$

$$T_{C_i} = -\frac{R_i T}{R} \tag{F-21}$$

Substituting Eqs. (F-19) through (F-21) into Eqs. (F-10) through (F-12) and Eqs. (F-15) through (F-17) yields the following results.

$$\psi_{iP} = (\phi'_{iT}\,\sigma'_i + \phi'_i\,\sigma'_{iT})\,\frac{T}{P} \tag{F-22}$$

$$\psi_{i\rho} = \phi'_i\,\sigma'_{i\rho} - (\phi'_{iT}\,\sigma'_i + \phi'_i\,\sigma'_{iT})\,\frac{T}{\rho} \tag{F-23}$$

$$(\psi_k)_{C_i} = (\phi'_k)_{C_i}\,\sigma'_k + \phi'_k(\sigma'_k)_{C_i} - (\phi'_{kT}\,\sigma'_k + \phi'_k\,\sigma'_{kT})\,\frac{R_i T}{R} \tag{F-24}$$

$$\sigma_{iP} = \sigma'_{iT}\,\frac{T}{P} \tag{F-25}$$

$$\sigma_{i\rho} = \sigma'_{i\rho} - \sigma'_{iT}\,\frac{T}{\rho} \tag{F-26}$$

$$(\sigma_k)_{C_i} = (\sigma'_k)_{C_i} - \sigma'_{kT}\,\frac{R_i T}{R} \tag{F-27}$$

Substituting Eqs. (F-22) through (F-27) into Eqs. (F-1) through (F-3) results in the following equations for K_3, K_4, and J_i.

$$K_3 = - h_4 \frac{T}{P} \sum_{i=1}^{n} \phi'_{iT} \, \sigma'_i - \frac{T}{P} \sum_{i=1}^{n} (h_4 \phi'_i + g_i) \phi'_{iT} \tag{F-28}$$

$$K_4 = h_4 \frac{a^2}{P} \sum_{i=1}^{n} \psi'_i + \frac{1}{\rho} \sum_{i=1}^{n} (h_4 a^2 a_i + g_i) \sigma'_i -$$

$$- a^2 \frac{T}{P} \sum_{i=1}^{n} \left[h_4 \phi'_{iT} \, \sigma'_i + (h_4 \phi'_i + g_i) \sigma'_{iT} \right] -$$

$$- \sum_{i=1}^{n} (h_4 \phi'_i + g_i) \sigma'_{i\rho} + h_4 \frac{T}{\rho} \sum_{i=1}^{n} \phi'_{iT} \sigma'_i +$$

$$+ \frac{T}{\rho} \sum_{i=1}^{n} (h_4 \phi'_i + g_i) \sigma'_{iT} \tag{F-29}$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} \left[(\phi'_k)_{C_i} - \frac{R_i T}{R} \phi'_{kT} \right] \sigma'_k -$$

$$- \sum_{k=1}^{n} (h_4 \phi'_k + g_k) \, (\sigma'_k)_{C_i} + \sum_{k=1}^{n} \frac{R_i T}{R} (h_4 \phi'_k + g_i) \sigma'_{kT} \tag{F-30}$$

All that remains to be done to obtain the final result is to evaluate the derivatives of ϕ'_i and σ'_i, defined by Eqs. (F-5) and (F-14) respectively, and substitute the results into Eqs. (F-28) through (F-30). From Eq. (F-5),

$$d\phi'_i = \gamma R_i dT + R_i T d\gamma - (\gamma-1) C_{Pi} dT - h_i d\gamma \tag{F-31}$$

$$d\phi'_i = [\gamma R_i - (\gamma-1) C_{Pi}] dT + [R_i T - h_i] d\gamma \tag{F-32}$$

The specific heat ratio γ is given by

$$\gamma = C_\rho / C_v \tag{F-33}$$

$$d\gamma = \frac{\gamma}{C_P} dC_P - \frac{\gamma}{C_v} dC_v \tag{F-34}$$

$$C_P = \sum_{i=1}^{n} C_{Pi} C_i \tag{F-35}$$

$$dC_P = \sum_{i=1}^{n} C_{Pi} dC_i \tag{F-36}$$

$$C_v = \sum_{i=1}^{n} C_{vi} C_i \tag{F-37}$$

$$dC_v = \sum_{i=1}^{n} C_{vi} dC_i \tag{F-38}$$

Combining Eqs. (F-34) through (F-38) gives the following result for $d\gamma$.

$$d\gamma = \gamma \sum_{k=1}^{n} a_k dC_k \tag{F-39}$$

where a_i is defined by Eq. (24) and is equal to

$$a_i = \frac{1}{C_P} (C_{Pi} - \gamma C_{vi}) \tag{F-40}$$

The coefficient of dT in Eq. (F-32) can be rearranged as follows.

$$[\gamma R_i - (\gamma-1)C_{Pi}] = C_{Pi} - \gamma C_{vi} = C_P a_i \tag{F-41}$$

Combining Eqs. (F-32), (F-39) and (F-41) gives

$$d\phi_i' = C_P a_i dT + (R_i T - h_i) \gamma \sum_{k=1}^{n} a_k dC_k \tag{F-42}$$

$$\phi'_{iT} = C_p a_i \tag{F-43}$$

$$(\phi'_k)_{C_i} = (R_k T - h_k) a_i \tag{F-44}$$

The derivatives of σ'_i can be obtained by differentiating Eq. (F-14).

$$\sigma'_{i\rho} = \frac{W_i}{\rho} \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left[K_{fr} \sum_{j=1}^{n} \nu'_{jr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - K_{rr} \sum_{j=1}^{n} \nu''_{jr} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right] \tag{F-45}$$

$$\sigma'_{iT} = W_i \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left[\frac{dK_{fr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - \frac{dK_{rr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right] \tag{F-46}$$

$$(\sigma'_k)_{C_i} = \frac{W_k}{C_i} \sum_{r=1}^{N} (\nu''_{kr} - \nu'_{kr}) \left[K_{fr} \nu'_{ir} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu'_{jr}} - K_{rr} \nu''_{ir} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j} \right)^{\nu''_{jr}} \right] \tag{F-47}$$

Substituting Eqs. (F-43) through (F-47) into Eqs. (F-28) through (F-30) results in the following final form of the parameters K_3, K_4, and J_i. Wherever ψ'_i and σ'_i appear in these equations, they have been replaced by ψ_i and σ_i by means of Eqs. (F-6) and (F-13) respectively.

$$K_3 = - h_4 \frac{C_pT}{P} \sum_{i=1}^{n} a_i\sigma_i - \frac{T}{P} \sum_{i=1}^{n} (h_4\phi_i + g_i) W_i \times$$

$$\times \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left[\frac{dK_{fr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu'_{jr}} - \frac{dK_{rr}}{dT} \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu''_{jr}}\right] \qquad \text{(F-48)}$$

$$K_4 = \frac{1}{\rho} \sum_{i=1}^{n} g_i\sigma_i + h_4 \frac{a^2}{P} \sum_{i=1}^{n} \psi_i - \frac{1}{\rho} \sum_{i=1}^{n} (h_4\phi_i + g_i)W_i \times$$

$$\times \sum_{r=1}^{N} (\nu''_{ir} - \nu'_{ir}) \left\{\left[K_{fr} \sum_{j=1}^{n} \nu'_{jr} + (\gamma-1)T \frac{dK_{fr}}{dT}\right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu'_{jr}} - \right.$$

$$\left. - \left[K_{rr} \sum_{j=1}^{n} \nu''_{jr} + (\gamma-1)T \frac{dK_{rr}}{dT}\right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu''_{jr}}\right\} \qquad \text{(F-49)}$$

$$J_i = g_i \frac{\rho v}{y} - h_4 \sum_{k=1}^{n} \left[\gamma(R_kT - h_k)a_i + \frac{C_pR_iT}{R} a_k\right] \sigma_k -$$

$$- \sum_{k=1}^{n} (h_4\phi_k + g_k)W_k \sum_{r=1}^{N} (\nu''_{kr} - \nu'_{kr}) \left\{\left[\frac{1}{C_i} K_{fr}\nu'_{ir} - \right.\right.$$

$$\left. - \frac{R_iT}{R} \frac{dK_{fr}}{dT}\right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu'_{jr}} - \left[\frac{1}{C_i} K_{rr}\nu''_{ir} - \right.$$

$$\left.\left. - \frac{R_iT}{R} \frac{dK_{rr}}{dT}\right] \prod_{j=1}^{n} \left(\frac{\rho C_j}{W_j}\right)^{\nu''_{jr}}\right\} \qquad (i=1,..,n) \qquad \text{(F-50)}$$