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AN ANALYSIS OF INTERNAL SUPERSONIC FLOWS

WITH DIFFUSION, DISSIPATION AND

HYDROGEN-AIR COMBUSTION

By

S. Dash

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BY

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LIST OF SYMBOLS

C_p	=	C_p^*/C_{p_∞} specific heat
J	=	0 for two dimensional flow, 1 for axisymmetric flow
L^*	=	reference length (throat radius)
Le	=	Lewis number
M	=	Mach number
m_i	=	molecular weight of ith specie
n	=	distance normal to streamline
P	=	$P^*/\rho_\infty u_\infty^2$ pressure
Pr	=	Prandtl number
q	=	q^*/u_∞ velocity
R	=	mixture gas constant
Re	=	free stream Reynolds number $\frac{\rho_\infty u_\infty L^*}{\mu_\infty}$
R_0	=	universal gas constant
$S_{1,2,3,i}$	=	forcing function terms
T	=	T^*/T_∞ temperature
W	=	average molecular weight of mixture
w_i	=	chemical production terms
x	=	x^*/L^* axial distance
y	=	y^*/L^* radial distance
α_i	=	mass fraction of ith specie
γ	=	ratio of specific heats
θ	=	flow inclination relative to axis

LIST OF SYMBOLS (Continued)

ρ = ρ^*/ρ_∞ density

μ_f = Mach angle

μ = viscosity

ψ = stream function

$*$ = dimensional variables

∞ = free stream conditions (dimensional)

f = frozen state

I. INTRODUCTION

The analysis of non-uniform flows having chemical reactions is considered. Both combustion and diffusive effects can significantly alter the wave pattern in a supersonic flow field, and hence, generate significant pressure gradients in both the axial and radial directions. The induced pressure field, in turn, can substantially influence ignition delay and reaction times as well as the velocity distribution. In analyzing such flow fields, the effects of finite rate chemistry, mixing and wave propagation must be intimately coupled. The overall pressure distribution in the flow field results from both pressures induced locally by mixing and combustion as well as pressures induced by boundary effects such as wall curvature.

A technique had been proposed (Reference (1)) where flows are analyzed taking into account pressure gradients both along and normal to streamlines, while the effects of transport properties are assumed to be a function only of gradients normal to the streamlines. This type of approach has been applied to the analyses of combustion phenomena controlled by mixing in References (2) and (3), and to the analyses of viscous flow problems in the presence of walls in Reference (4).

Only supersonic flow fields will be considered in the analysis. This allows us to use a modified characteristic calculation accounting for diffusion normal to the streamlines and finite rate chemistry along them, with pressure variations both along and normal to the streamlines. The resulting system of equations as presented in Section II, exhibits a dual mathematical nature. That is, the system is of a hyperbolic-parabolic nature. Were the flow to contain imbedded subsonic regions, the distinctive feature of hyperbolic or parabolic equations, namely the lack of upstream influence, would be lost and a marching type scheme could not be employed.

A numerical program has been generated which calculates non-uniform supersonic flows with diffusive and dissipative effects within two dimensional or axisymmetric nozzles. The chemistry is either frozen or finite-rate, for the hydrogen-air system based on the method and scheme described in References (8) and (9).

Since the profile to be expanded through the nozzle is non-uniform, the nozzle contour yielding flow parallel to the axis and constant pressure at the exit section may deviate substantially from a contour whose design is based on a uniform profile. The design of a two dimensional or axisymmetric nozzle, based on a non-uniform incoming flow has

been performed as described in Reference (5). Use of such a contour enables the distinguishing of viscous and chemical effects from those effects due solely to the rotationality of the flow.

The analysis performed is applicable to all viscous, reacting flow fields bounded or unbounded, if the flow remains supersonic and shock free in the domain considered. The viscous characteristics approach has been employed in the study of hypersonic viscous interaction (Reference (4)), where the supersonic portion of the boundary layer and rotational shock layer are solved by the viscous characteristics technique. The supersonic region is bounded below by the subsonic portion of the boundary layer and above by a shock. No chemical effects have been considered in that analysis.

A very important future application of the viscous characteristic method lies in the area of fuel injector and combustor analysis and design. To analyze these areas, where a large amount of heat is released over a relatively small region, the current program would require modifications to allow for the possibility (or more likely, probability) of enclosed subsonic regions and imbedded shock waves.

The application of this method to fuel injector calculations

would necessarily involve imbedded shocks, even for the case of tangential injection. When the fuel and air ignite a significant streamline deflection is generated, which is initially of the order of 20° to 30° for hydrogen-air combustion. If the Mach numbers of both fuel and air are sufficiently high, this deflection leads to the formation of oblique shocks on either side of the combustion zone propagating into both the fuel and air streams, with supersonic flow behind both these waves. For lower fuel or air Mach numbers, this initial deflection can produce local regions of subsonic flow behind these shocks. In addition, regions of subsonic flow will always be encountered when air and fuel initially come together, due to the air and fuel boundary layers existing on either side of the splitter plate. The inclusion of this wake region is quite important since the low velocity in the core greatly increases the residence time while the high core temperature produced by boundary layer heating may spark ignition. The failure to include the wake as part of the initial profile can lead to a poor prediction of the area of ignition and hence a misleading streamline and wave pattern.

In designing a combustor for supersonic combustion, use of a parabolic mixing analysis with chemical reactions completely ignores the complex wave pattern occurring within the combustor. The viscous characteristic approach can be intelligently

employed in combustor design to trace Mach waves through the viscous reacting flow field and to obtain wall contours in a manner consistent with the streamline deflections produced by the local regions of combustion.

To perform calculations of injector and burner flow fields, the viscous characteristics program must be expanded to handle local imbedded subsonic regions as well as shock formation and propagation in regions of highly viscous and reacting flow. A program capable of analyzing such complex flow situations would appear to be of significant use in the analysis of both scramjet and rocket interior flow fields.

Stability and accuracy criterion govern the step sizes employed in the numerical scheme. These limitations are presented in Section III. The overall numerical analysis is presented in Section IV, including the difference form of the equations, overall numerical procedure, and a method for uncoupling diffusion and chemistry. Some sample calculations are described in Section V, including the comparison of a non-uniform inviscid flow with its viscous counterpart, and the specific effects generated by combustion on the overall pressure distribution and wave pattern.

The computer program is available from COSMIC (Computer Software Management and Information Center) at the University of Georgia. Inquiries concerning the program should be addressed to:

COSMIC
Barrow Hall
University of Georgia
Athens, Georgia 30601

and should refer to program number LAR-10793.

II. BASIC EQUATIONS

The equations of motion, written below, govern flow fields where gradients normal to streamlines are much larger than gradients along streamlines. They are evolved from the full Navier-Stokes equations by retaining those diffusive terms depending only on gradients normal to streamlines, the normal momentum equation being retained in inviscid form. Only two dimensional or axisymmetric flows are considered.

In an intrinsic coordinate system, with s along and n normal to the streamlines, the resulting equations in non-dimensional form are as follows:

Global Continuity:

$$\frac{\partial(\rho q)}{\partial s} + \rho q \frac{\partial \theta}{\partial n} + \frac{J \rho q}{y} \sin \theta = 0 \quad (1)$$

S-Momentum:

$$\rho q \frac{\partial q}{\partial s} + \frac{\partial p}{\partial s} = \frac{1}{R_e} \left[\frac{\partial}{\partial n} \left(\mu \frac{\partial q}{\partial n} \right) + \frac{J}{y} \cos \theta \mu \frac{\partial q}{\partial n} \right] \quad (2)$$

N-Momentum:

$$\rho q^2 \frac{\partial \theta}{\partial s} + \frac{\partial p}{\partial n} = 0 \quad (3)$$

Energy:

$$C_p \rho q \frac{\partial T}{\partial s} - q \frac{\partial p}{\partial s} = \frac{1}{R_e(\gamma_\infty - 1)M_\infty^2}$$

$$\left[\frac{\partial}{\partial n} \left(\frac{\mu C_p}{P_r} \frac{\partial T}{\partial n} \right) + \frac{J}{y} \cos \theta \frac{C_p \mu}{P_r} \frac{\partial T}{\partial n} + \frac{\mu L_e}{P_r} \frac{\partial T}{\partial n} \sum C_{p_i} \frac{\partial \alpha_i}{\partial n} \right. \\ \left. + (\gamma_\infty - 1)M_\infty^2 \mu \left(\frac{\partial q}{\partial n} \right)^2 \right] - \sum \dot{w}_i h_i \quad (4)$$

Species Conservation:

$$\rho q \frac{\partial \alpha_i}{\partial s} = \frac{1}{R_e} \left[\frac{\partial}{\partial n} \left(\frac{L_e \mu}{P_r} \frac{\partial \alpha_i}{\partial n} \right) + \frac{J}{y} \frac{L_e}{P_r} \cos \theta \mu \frac{\partial \alpha_i}{\partial n} \right] \\ + \dot{w}_i \quad (5)$$

State:

$$p = \frac{W_\infty \rho T}{\gamma_\infty M_\infty^2 W} \quad (6)$$

where

$$W = \left[\sum \frac{\alpha_i}{m_i} \right]^{-1}$$

For supersonic flow fields, the above system of partial differential equations, generally termed the "viscous-inviscid" equations, exhibits features characteristic of both hyperbolic and parabolic systems. The numerical scheme employed in this analysis couples a characteristic network with a boundary layer type network to yield a coupled solution.

The characteristic solution feels the effects of diffusion and finite-rate chemistry by treating the diffusive and chemistry terms as forcing functions in the compatibility relation along characteristics.

For convenience, let us denote the diffusive terms appearing in the right hand sides of Equations (2), (4) and (5) as follows:

$$S_1 = \frac{1}{R_e} \left[\frac{\partial}{\partial n} \left(\mu \frac{\partial q}{\partial n} \right) + \frac{J}{y} \cos \theta \mu \frac{\partial q}{\partial n} \right] \quad (7)$$

$$S_2 = \frac{1}{R_e (\gamma_\infty - 1) M_\infty^2} \left[\frac{\partial}{\partial n} \left(\frac{\mu C_p}{P_r} \frac{\partial T}{\partial n} \right) + \frac{J}{y} \cos \theta \frac{\mu C_p}{P_r} \frac{\partial T}{\partial n} \right. \\ \left. + \mu \frac{L_e}{P_r} \frac{\partial T}{\partial n} \sum C_{p_i} \frac{\partial \alpha_i}{\partial n} + (\gamma_\infty - 1) M_\infty^2 \mu \left(\frac{\partial q}{\partial n} \right)^2 \right] \quad (8)$$

$$S_{3_i} = \frac{1}{R_e} \left[\frac{\partial}{\partial n} \left(\frac{L_e \mu}{P_r} \frac{\partial \alpha_i}{\partial n} \right) + \frac{J}{y} \frac{L_e}{P_r} \cos \mu \frac{\partial \alpha_i}{\partial n} \right] \quad (9)$$

Equations (2), (4) and (5) may now be rewritten

$$\rho q \frac{\partial q}{\partial s} + \frac{\partial p}{\partial s} = S_1 \quad (10)$$

$$C_p \rho q \frac{\partial T}{\partial s} - q \frac{\partial p}{\partial s} = S_2 - \sum \dot{w}_i h_i \quad (11)$$

$$\rho q \frac{\partial \alpha_i}{\partial s} = S_{3_i} + \dot{w}_i \quad (12)$$

The system of Equations (1), (3), (6), (10), (11) and (12) differ from the non-reacting inviscid flow equations only by the terms appearing on the right of Equations (10), (11) and (12). By treating these terms as forcing functions, the characteristic directions remain those of the inviscid system, namely the frozen Mach lines ($C_{\pm}$)

$$\frac{dy}{dx} = \tan (\theta \pm \mu_f) \quad (13)$$

and streamlines are defined by the relation

$$\frac{dy}{dx} = \tan \theta \quad (14)$$

By algebraic manipulation, the compatibility relation along a $C_{\pm}$ characteristic may be obtained (as described in Appendix I).

$$\frac{\sin \mu_f \cos \mu_f}{\gamma_f p} dp \pm d\theta + \left[\frac{J \sin \theta}{y} + \right.$$

$$\frac{S_1}{\rho q^2} - \frac{(\gamma_f - 1)}{\gamma_f p q} S_2 + \frac{\gamma_f - 1}{\gamma_f (\gamma_\infty - 1) M_{\infty p q}^2} \Sigma \dot{w}_i h_i - \quad (15)$$

$$\frac{W}{\rho q} \Sigma \left(\frac{S_{3i}}{m_i} + \frac{\dot{w}_i}{m_i} \right) \left[\frac{\sin \mu_f}{\cos(\theta \pm \mu_f)} dx = 0 \right.$$

III. STABILITY REQUIREMENTS

The grid for the overall numerical computation is depicted in Figure (1). Properties are specified at the mesh points

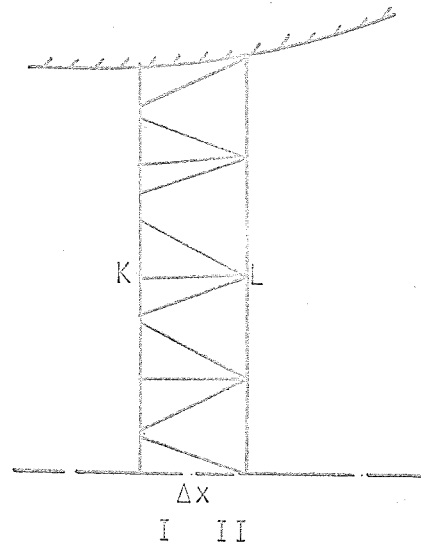


FIGURE 1. NETWORK FOR NUMERICAL COMPUTATION

K at station I and desired at the mesh points L at station II, the line K-L being a streamline. The distance between stations I and II is limited by three separate criteria, namely characteristic stability, parabolic stability and accuracy for the finite-rate chemistry calculation. In the scheme employed, the finite-rate chemistry and diffusion are uncoupled as will be subsequently described. The chemistry requirements are then met by subdividing the streamline K-L into sub-intervals Δs_{chem} each satisfying the chemistry requirements, thus chemistry does not effect the overall step size Δx . The maximum allowable step size satisfying char-

acteristic stability is obtained by intersecting the up and down running characteristics emanating from the mesh points K, and selecting the smallest distance marched as Δx_{char} .

This procedure is depicted in Figure (2).

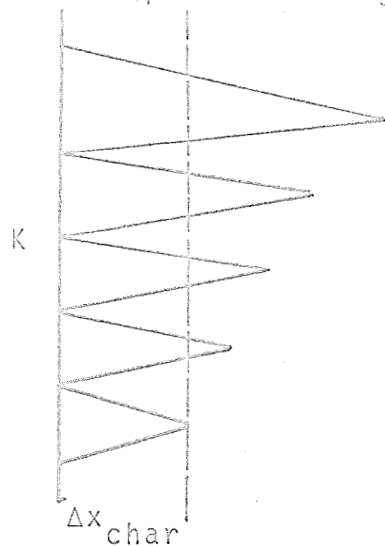


FIGURE 2. CHARACTERISTIC STEP SIZE.

Parabolic stability arises from solving the s-momentum, energy and species conservation equations numerically along the streamlines K-L, by an explicit marching scheme, derivatives being made by a 3 point finite difference formula. For problems of interest $P_r \leq 1$ and $L_e \geq 1$, hence the species conservation equation dictates the step size criterion. In the scheme employed, the assumption is made that derivatives normal to the streamlines may be approximated by derivatives in the radial direction. This assumption is not crucial to the numerical scheme, and the actual derivatives normal to the streamlines could be calculated for significant streamline deflec-

tions.

For an explicit scheme, using a standard 3 point finite difference formulation with equal step sizes in the y direction, the step size Δs_{K-L} is limited by the stability requirement (Reference (6)).

$$\Delta s_{K-L} \leq \frac{1}{2} \rho q \frac{P_r R_e}{\mu L_e} \Delta y^2 \quad (16)$$

imposed from the species conservation equation. In the scheme used in this analysis, the mesh points K are not equally spaced in the y direction, hence being conservative the smaller Δy is used. The step size Δx_{par} is found by choosing the minimum Δs_{K-L} for all streamlines K-L based on properties at station I and hence

$$\Delta x_{par} \leq \frac{1}{2} \rho q \cos \theta \frac{P_r R_e}{\mu L_e} \Delta y^2 \quad (17)$$

The step size in the computation is then the smaller of Δx_{par} and Δx_{char} .*

*It was found in the numerical computations that the use of the step size criterion in Equation (17) still led to instabilities, particularly near the axis in axisymmetric cases. Use of $1/2 \Delta x_{par}$ made the computation stable.

IV. NUMERICAL ANALYSIS(a) Difference Form of Characteristic Equations.

Referring to Figure (3), let

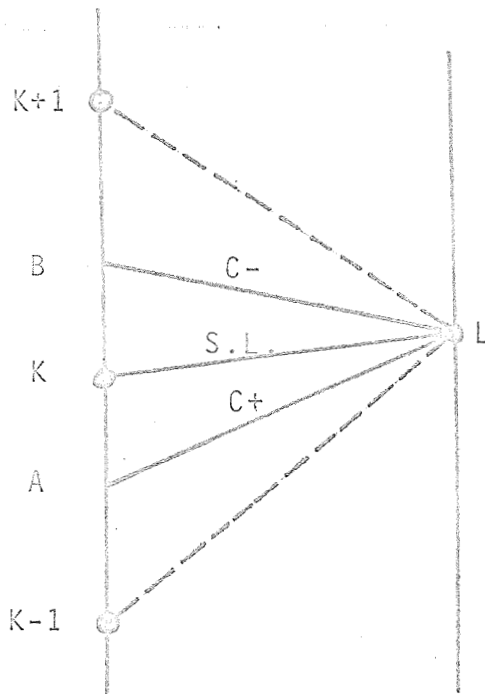


FIGURE 3. NUMERICAL GRID

$$M_1 = \alpha \tan (\theta + \mu_+) _A + \beta \tan (\theta + \mu_+) _L \quad (18a)$$

$$M_2 = \alpha \tan (\theta - \mu_+) _B + \beta \tan (\theta - \mu_+) _L \quad (18b)$$

hence along a C_+ characteristic (AL),

$$\frac{y_L - y_A}{\Delta x} = M_1 \quad (19a)$$

and along a C_- characteristic (BL),

$$\frac{y_L - y_B}{\Delta x} = M_2 \quad (19b)$$

The terms α and β are used as artifices in averaging properties across the characteristics. In the first iteration (a linearized calculation), all coefficients appearing in the characteristic relations are evaluated at the initial station, while in subsequent iterations they are averaged across the characteristics. To achieve this in the numerical scheme, α is set equal to one and β to zero in the first iteration, while both α and β are set equal to one-half in subsequent iterations.

Let

$$A_1 = \alpha \left(\frac{\sin \mu_c \cos \mu_r}{\gamma p} \right)_A + \beta \left(\frac{\sin \mu_c \cos \mu_r}{\gamma p} \right)_L \quad (20a)$$

$$B_1 = \alpha \left(\frac{\sin \mu_c \cos \mu_r}{\gamma p} \right)_B + \beta \left(\frac{\sin \mu_c \cos \mu_r}{\gamma p} \right)_L \quad (20b)$$

First and second derivatives, with respect to y , for the variables q , T and α_i , are calculated at all the mesh points K on the initial line using the standard finite difference equations

$$\left(\frac{\partial F}{\partial y}\right)_K = \frac{F_{K+1} \frac{\Delta y_1}{\Delta y_2} - F_K \left(\frac{\Delta y_1}{\Delta y_2} - \frac{\Delta y_2}{\Delta y_1}\right) - F_{K-1} \frac{\Delta y_2}{\Delta y_1}}{(\Delta y_1 + \Delta y_2)} \quad (21)$$

and

$$\left(\frac{\partial^2 F}{\partial y^2}\right)_K = \frac{2(F_{K+1} \frac{\Delta y_1}{\Delta y_1 + \Delta y_2} - F_K + F_{K-1} \frac{\Delta y_2}{\Delta y_1 + \Delta y_2})}{\Delta y_1 \Delta y_2} \quad (22)$$

where

$$\Delta y_1 = y_K - y_{K-1}$$

and

$$\Delta y_2 = y_{K+1} - y_K$$

Let

$$S_{1AL} = \frac{1}{2} \left[S_{1A} + (\alpha - \beta) S_{1K} + 2\beta S_{1L} \right] \quad (23a)$$

$$S_{1BL} = \frac{1}{2} \left[S_{1B} + (\alpha - \beta) S_{1K} + 2\beta S_{1L} \right] \quad (23b)$$

$$S_{2AL} = \frac{1}{2} \left[S_{2A} + (\alpha - \beta) S_{2K} + 2\beta S_{2L} \right] \quad (24a)$$

$$S_{2_{BL}} = \frac{1}{2} \left[S_{2_B} + (\alpha - \beta) S_{2_K} + 2\beta S_{2_L} \right] \quad (24b)$$

$$S_{3_{i_{AL}}} = \frac{1}{2} \left[S_{3_{i_A}} + (\alpha - \beta) S_{3_{i_K}} + 2\beta S_{3_{i_L}} \right] \quad (25a)$$

$$S_{3_{i_{BL}}} = \frac{1}{2} \left[S_{3_{i_B}} + (\alpha - \beta) S_{3_{i_K}} + 2\beta S_{3_{i_L}} \right] \quad (25b)$$

The above diffusive terms, appearing in the characteristic compatibility relation (Equation (15)) consists of combinations of first and second derivatives of q , T and α_i as in Equations (7), (8) and (9).

Consider the term S_{1_A} appearing in Equation (23a). Expanding Equation (7), we obtain

$$S_{1_A} = \frac{1}{Re} \left[\left(\mu \frac{\partial^2 q}{\partial n^2} \right) + \frac{\partial u}{\partial n} \frac{\partial q}{\partial n} + \frac{j}{y} \cos \theta \mu \frac{\partial q}{\partial n} \right]_A$$

Properties and derivatives required at point A, are found by linearly interpolating between the values stored at the mesh points K-1 and K. The term $S_{1_{AL}}$ represents the average value of S_1 along the C_+ characteristic AL. In the first iteration, properties at L are unknown, and the value at L is approximated by the value at K, based on the assumption that changes along streamlines are much smaller than changes normal to them for

the diffusive terms. Hence

$$S_{1AL} \approx \frac{1}{2} (S_{1A} + S_{1K})$$

For successive iterations where properties and derivatives are known at L,

$$S_{1AL} = \frac{1}{2} (S_{1A} + S_{1L})$$

The above remarks pertain to all the diffusive terms (Equations (23) - (25)) where the averaging used is indicated by use of α and β coefficients.

Let

$$A_2 = \left[\frac{S_1}{\rho q^2} - \frac{(\gamma_f - 1)}{\gamma_f p q} S_2 - \frac{W}{\rho q} \sum \frac{S_{3i}}{m_i} \right]_{AL} \quad (26a)$$

$$B_2 = \left[\frac{S_1}{\rho q^2} - \frac{(\gamma_f - 1)}{\gamma_f p q} S_2 - \frac{W}{\rho q} \sum \frac{S_{3i}}{m_i} \right]_{BL} \quad (26b)$$

$$A_3 = \left[\frac{\gamma_f^{-1}}{\gamma_f (\gamma_\infty - 1) M_{\infty}^2 p q} \sum \dot{w}_i h_i - \frac{W}{\rho q} \sum \frac{\dot{w}_i}{m_i} \right]_{AL} \quad (27a)$$

$$B_3 = \left[\frac{\gamma_f^{-1}}{\gamma_f (\gamma_\infty - 1) M_{\infty}^2 p q} \sum \dot{w}_i h_i - \frac{W}{\rho q} \sum \frac{\dot{w}_i}{m_i} \right]_{BL} \quad (27b)$$

$$A_4 = \alpha \frac{\sin \mu_c}{\cos(\theta + \mu_c)}_A + \beta \frac{\sin \mu_c}{\cos(\theta + \mu_c)}_L \quad (28a)$$

$$B_4 = \alpha \frac{\sin \mu_c}{\cos(\theta - \mu_c)}_B + \beta \frac{\sin \mu_c}{\cos(\theta - \mu_c)}_L \quad (28b)$$

Then along $C \pm$ characteristics the compatibility equations in difference form, may be written

$$A_1(p_C - p_A) + \theta_C - \theta_A + \left[\frac{J \sin \theta}{y}_{AC} + A_2 + A_3 \right] A_4(x_C - x_A) = 0 \quad (29)$$

along (AL)

and

$$B_1(p_C - p_A) - \theta_C + \theta_B + \left[\frac{J \sin \theta}{y}_{BC} + B_2 + B_3 \right] B_4(x_C - x_B) = 0 \quad (30)$$

along (BL).

(b) Numerical Procedure. All properties at station I are specified at the mesh points K, the spacing between these points not necessarily being uniform. The point L is located, in a linear approximation, by the streamline relation $y_L = y_K + (\tan \theta_K) \Delta x$ and hence $\Delta s_{KL} = \Delta x / \cos \theta_K$.

The chemistry and diffusion are uncoupled by the following procedure, first devised by A. Ferri et. al. (Reference (2)).

Let

$$\alpha_i = \alpha_{iD} + \alpha_{iC}$$

$$T = T_D + T_C$$

Then the species conservation equation may be split into the following two equations:

$$\rho q \frac{\partial \alpha_{iC}}{\partial s} = \dot{w}_i \quad (31)$$

and

$$\rho q \frac{\partial \alpha_{iD}}{\partial s} = S_{3i} \quad (32)$$

while the energy equation splits into

$$C_p \rho q \frac{\partial T_C}{\partial s} = - \sum \dot{w}_i h_i \quad (33)$$

and

$$c_p \rho q \frac{\partial T_D}{\partial s} = q \frac{\partial p}{\partial s} + S_2 \quad (34)$$

Equations (31) and (33) pertain to a premixed flow with finite-rate chemistry while Equations (32) and (34) refer to purely diffusive flows with pressure gradients.

Referring to Figure (4),

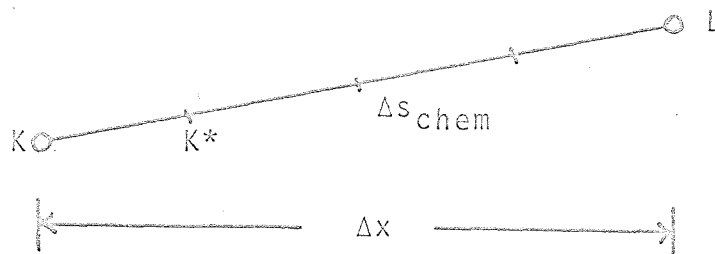


FIGURE 4. SUBDIVISION OF STREAMLINE INTO CHEMICAL STEPS

an inviscid one dimensional finite-rate chemistry calculation is performed along the streamline K-L. The chemistry step size is limited by a time step criterion Δt . This is translated into a chemical step size Δs_{chem} by the relation

$$\Delta s_{chem} = \Delta t q^* \quad \text{where } q^* = u_{\infty} q.$$

The interval K-L is then subdivided into a finite number of chemical steps. The assumption is made that the pressure is constant for the interval K-L, as far as the chemistry calcula-

tions are concerned. The chemistry calculation first proceeds from K to K*, yielding $\Delta\alpha_{iC_{K-K^*}}$ and $\Delta T_{C_{K-K^*}}$.

New properties (induced by chemistry) are then calculated at K*, the pressure being fixed as that at K. Marching in this manner, $\Delta T_{C_{K-L}}$ and $\Delta\alpha_{iC_{K-L}}$ induced by chemistry are obtained, as well as the production rates $\dot{w}_{iK}$ and $\dot{w}_{iL}$, which will be required in the characteristic calculation. The details of the chemistry have been described in Reference (8) and (9). The calculation described above is performed for all streamlines K-L in the grid, the values $\Delta\alpha_{iC}$, ΔT_C , $\dot{w}_{iK}$ and $\dot{w}_{iL}$, being stored at the mesh points, as their values will be required in the subsequent calculations.

Points A and B are located by interpolating between the mesh points at station I using relations

$$y_A = y_L - M_1 \Delta x$$

$$y_B = y_L - M_2 \Delta x$$

where

$$x_A = x_B = x_K$$

Properties (including the first and second derivatives of q, T

and α_i) are obtained at A and B by interpolation and hence the forcing function terms (Equations (23) through (25)) can be calculated.

Solving Equations (29) and (30), we obtain

$$P_C = (A_1 P_A + B_1 P_B + \theta_A - \theta_B - (A_5 + B_5) x_C + A_5 x_A + B_5 x_B) / (A_1 + B_1) \quad (35)$$

where

$$A_5 = (A_2 + A_3 + \frac{J \sin \theta}{y}) A_4 \quad \text{and} \quad B_5 = (B_2 + B_3 + \frac{J \sin \theta}{y}) B_4$$

and

$$\theta_C = \theta_A - A_1 (P_C - P_A) - A_5 (x_C - x_A) \quad (36)$$

Evaluating the forcing functions along the streamline K-L,

$$S_{1K-L} = \alpha S_{1K} + \beta S_{1L}$$

$$S_{2K-L} = \alpha S_{2K} + \beta S_{2L}$$

and

$$S_{3iK-L} = \alpha S_{3iK} + \beta S_{3iL}$$

we obtain q , T and α_i at L as follows:

From the S -momentum equation (Equation (2))

$$q_L = q_K + \frac{S_{1KL} \Delta x / (\alpha \cos \theta_K + \beta \cos \theta_L) - (P_L - P_K)}{\alpha(\rho q)_K + \beta(\rho q)_L} \quad (37)$$

from the energy equation (Equation (4))

$$T_L = T_K + \frac{(\gamma_\infty - 1) M_\infty^2 S_{2KL} \frac{\Delta x}{(\alpha \cos \theta_K + \beta \cos \theta_L)} + (\alpha q_K + \beta q_L)(P_L - P_K)}{\alpha(\rho q C_p)_K + \beta(\rho q C_p)_L} + \Delta T_{C_{KL}} \quad (38)$$

and from the species-diffusion equation (Equation (5))

$$\alpha_{iL} = \alpha_{iK} + \frac{S_{3iKL} \frac{\Delta x}{(\alpha \cos \theta_K + \beta \cos \theta_L)}}{\alpha(\rho q)_K + \beta(\rho q)_L} + \Delta \alpha_{iC_{KL}} \quad (39)$$

The remaining properties at L can then be evaluated as follows:

The average molecular weight is expressed by

$$W = \left[\sum \frac{\alpha_i}{m_i} \right]^{-1} \quad (40)$$

hence the mixtures gas constant is

$$R = \frac{R_0}{W} \quad (41)$$

From the equation of state, the density is

$$\rho = \frac{W_p}{T} \frac{\gamma_\infty M_\infty^2}{W_\infty} \quad (42)$$

The specific heat (frozen) is expressed by

$$c_p = \sum c_{p_i}(T) \alpha_i = \sum (\alpha_i \frac{\partial h_i(T)}{\partial T}) \quad (43)$$

Where $c_{p_i}(T)$ is a specified function of temperature, thermodynamic data being tabulated from Reference (7).

The ratio of specific heats is

$$\gamma_f = \frac{c_p}{c_p - R/c_{p_\infty}} \quad (44)$$

the Mach number is given by

$$M_f = \frac{M_\infty q}{\sqrt{T}} \left[\frac{\gamma_\infty R_\infty}{\gamma R} \right]^{1/2} \quad (45)$$

and hence the Mach angle is

$$\mu_f = \sin^{-1} \left(\frac{1}{M_f} \right) \quad (46)$$

(c) Axis Point Calculation. In axisymmetric flows, special consideration must be given to the compatibility relation in the vicinity of the axis, due to the indeterminacy of the term $\frac{\sin \theta}{y}$.

Consider the case indicated in Figure (5) where L is on the axis, and E is midway between B and L.

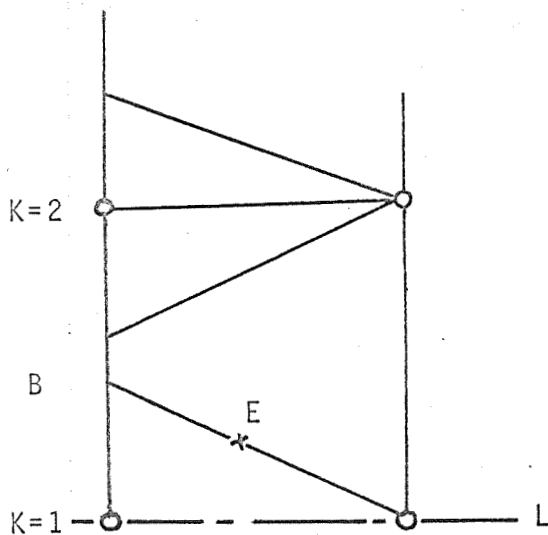


FIGURE 5. AXIS POINT CALCULATION

Note that at an axis point the expressions for first and second derivatives take the simple form

$$\left(\frac{\partial F}{\partial y}\right)_K = 0$$

and

$$\left(\frac{\partial^2 F}{\partial y^2}\right)_K = \frac{2(F_{K+1} - F_K)}{(\Delta y)^2}$$

where K is on the axis and $\Delta y = y_{K+1} - y_K$

The compatibility relation along BL rewritten here with θ_L equalling zero is:

$$B_1(P_L - P_B) + \theta_B + \left(\frac{J \sin \theta}{y} + B_2 + B_3\right) B_4(x_L - x_B) = 0$$

Consider the term $\frac{J \sin \theta}{y} B_4(x_L - x_B)$ which, upon expanding is

$$\left[\frac{J}{y} \frac{\sin \theta \sin \mu_f}{\cos(\theta - \mu_f)}\right]_E (x_L - x_B)$$

Near the axis $\sin \theta \sim \theta$

$$\frac{x_L - x_B}{y_E} = \frac{2(x_L - x_B)}{y_B} = \frac{-2}{\tan(\theta - \mu_f)_E}$$

hence we obtain

$$-2J \frac{\theta_E \sin \mu_E}{\sin(\theta - \mu_E)} = -J\theta_B \left[\frac{\sin \mu_E}{\sin(\theta - \mu_E)} \right]_E$$

hence the compatibility relation takes the form

$$B_1(P_L - P_B) + \theta_B(B_X) + (B_2 + B_3) B_4(x_L - x_B) = 0 \quad (47)$$

where

$$B_X = 1 - J \left[\alpha \left(\frac{\sin \mu_E}{\sin(\theta - \mu_E)} \right)_B + \beta \left(\frac{\sin \mu_E}{\sin(\theta - \mu_E)} \right)_C \right]$$

(d) Wall Point Calculation.

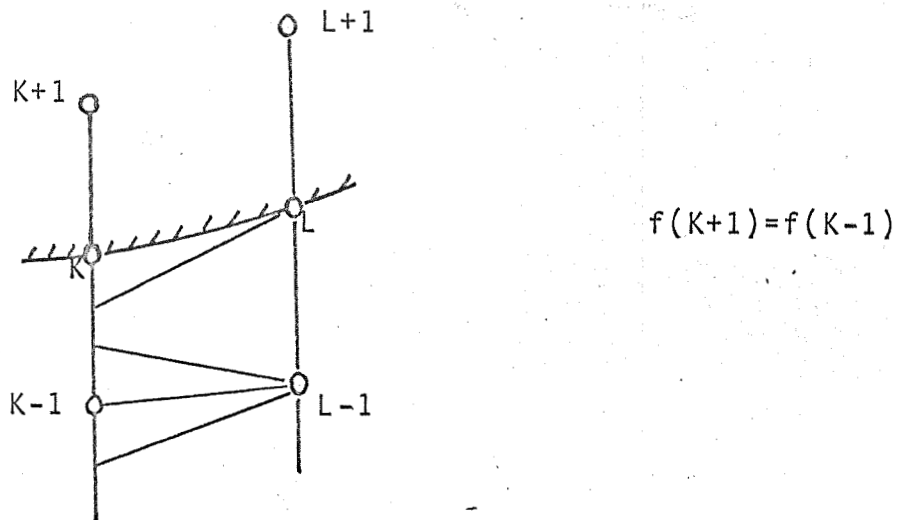


FIGURE 6. WALL POINT CALCULATION

The diffusive terms at the wall are evaluated by using a reflection principle, the effects of a wall boundary layer being neglected. This implies that the wall has no shear and is adiabatic and impermeable:

$$\frac{\partial q}{\partial y}_W = 0$$

$$\frac{\partial T}{\partial y} \Big|_W = 0$$

$$\frac{\partial \alpha_i}{\partial y_w} = 0$$

$$i = 1, \text{ NSP}$$

(48)

In difference form the wall conditions are obtained by setting properties (q , T and α_j) at $K+1$ equal to those of $K-1$, when K

is at the wall, and using the standard difference formulas for derivatives

With the wall contour specified, θ_C is known, hence the pressure P_C is obtained from Equation (30)

$$P_C = P_A + \frac{\theta_A - \theta_C + (A_2 + A_3 + \frac{J \sin \theta}{y}) A_4 (x_C - x_A)}{A_1} \quad (49)$$

with the coefficients A_1 , A_2 , A_3 and A_4 obtained as previously discussed.

Having obtained all the properties at point L, the characteristic calculation cannot at this point be repeated with averaged coefficients since the diffusive terms are not known at L. The procedure is to repeat the above set of calculations for all points at station II. Then the first and second derivatives can be obtained at all points. The calculation can then be repeated for all L points with properties averaged ($\alpha = \frac{1}{2}$, $\beta = \frac{1}{2}$). The pressures obtained in this second iteration are compared with the first set of pressures. If the change between the two iterations is substantial, the entire calculation is once more repeated until the change in pressures between two successive iterations is negligible. Several iterations may be necessary in regions of severe gradients, although in general, just two

iterations are required, as in an ordinary characteristic calculation.

V. SAMPLE CALCULATIONS

To demonstrate the method developed in this report, a nozzle contour was generated for the nonuniform entrance conditions depicted in Figure (7). This initial profile consists of a central core of hot H_2O and N_2 surrounded by an outer core of cooler air, the velocity and static pressure being uniform. The contour was obtained by the techniques developed in Reference (5) while the program generated based on this technique is described in Reference (10).

The initial profile was expanded through the designed nozzle using the viscous characteristic technique with frozen chemistry. The profiles at the exit plane are compared with those of the inviscid calculation, in Figure (8) the differences being due solely to diffusive and dissipative effects.

The free stream conditions in this calculation correspond to a Mach 8 air stream at an altitude of 100,000 feet. The free stream Reynolds number per unit length is 870,000 and both the Prandtl and Lewis numbers were taken as 1. The throat has a one inch radius and the turbulent viscosity was chosen as a constant equal to 1000 times the laminar value* at the entrance section. The velocity and temperature

* $(\mu = 1.35 \times 10^{-4} \frac{\text{lb-sec}}{\text{ft}^2})$

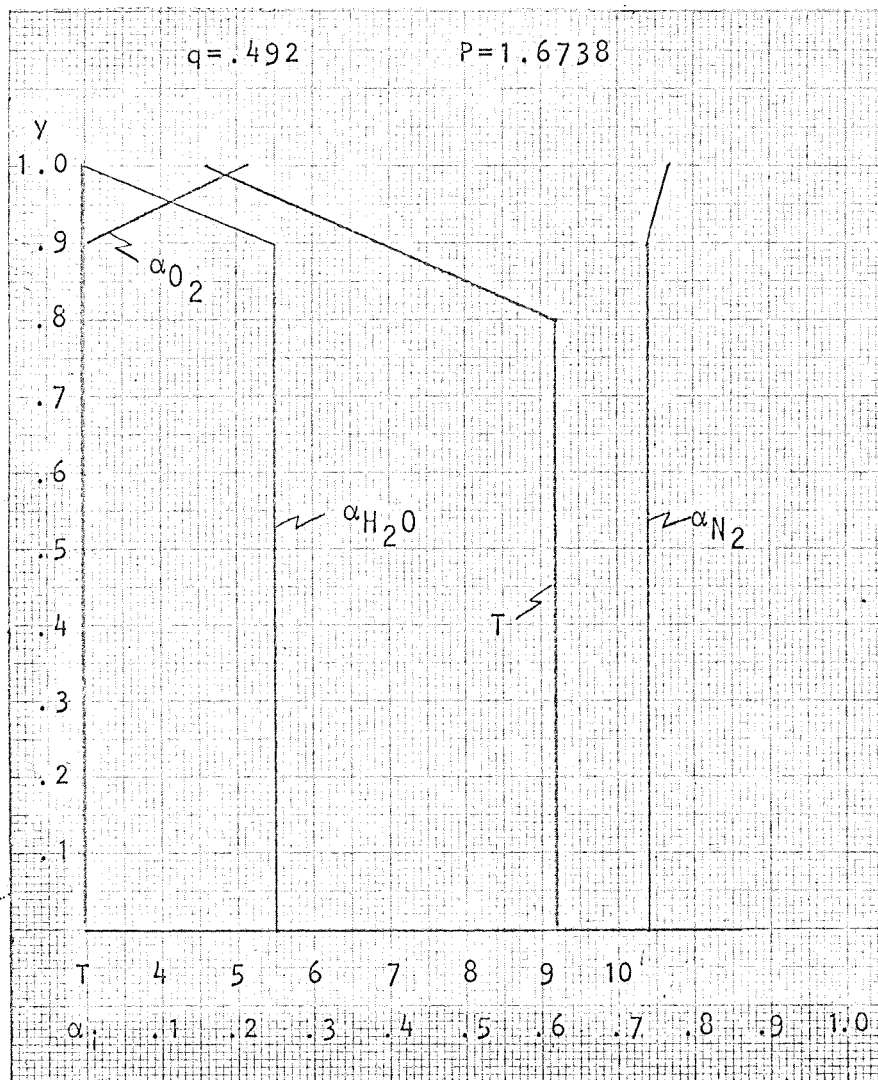


FIGURE 7. INITIAL PROFILES

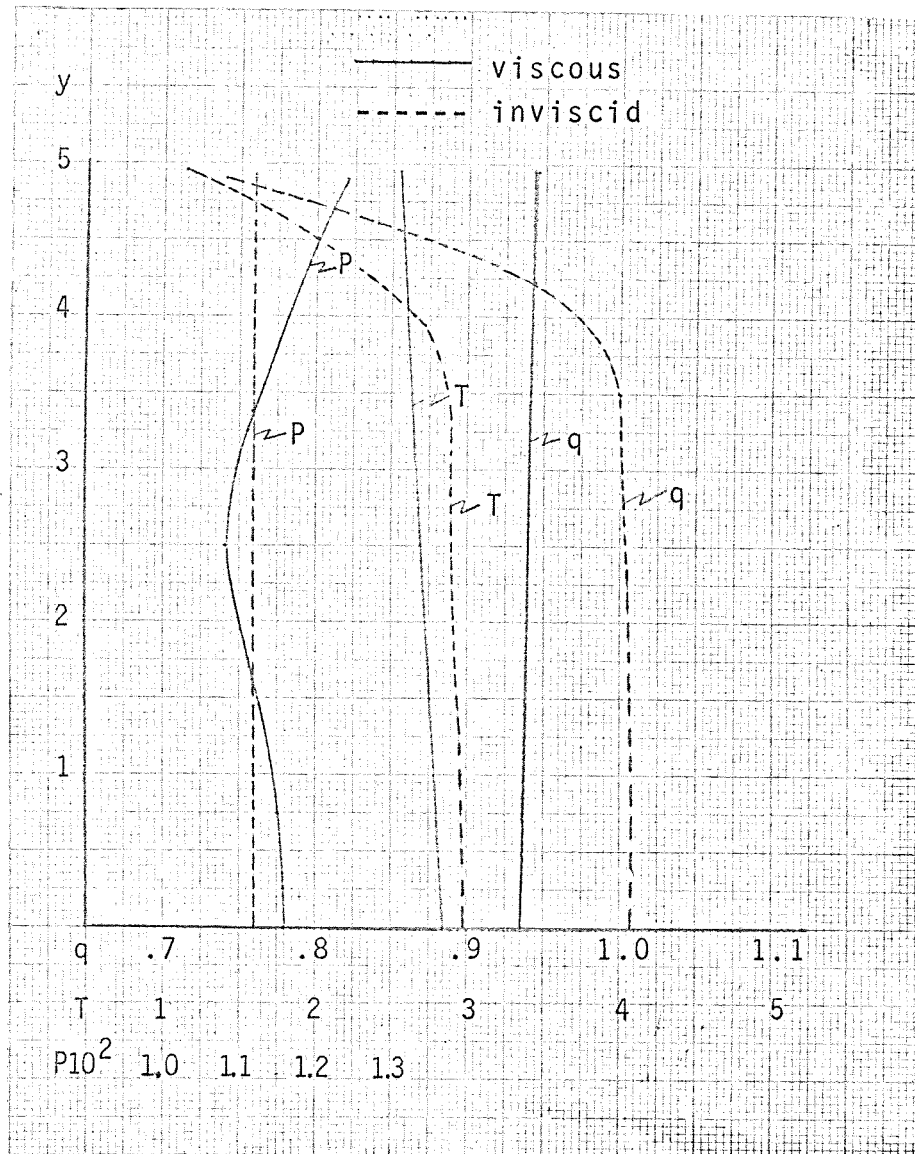


FIGURE 8. EXIT PROFILES

at the exit are essentially constant in the viscous case due to mixing, while the exit pressure is no longer uniform having the rather slight variation indicated.

The nozzle contour obtained is depicted in Figure (9) along with several streamlines and Mach lines from the viscous calculation. The dotted lines indicate the down-running characteristic yielding design pressure on the axis and the up-running characteristic downstream of which the pressure is uniform, obtained in the inviscid design calculation. The axial wall and axis Mach number distributions are shown in Figure (10) for the inviscid and viscous cases, while the corresponding pressure distributions are presented in Figure (11).

An additional viscous characteristics calculation was performed to show the viscous scaling effect of the throat radius on the problem. The radius was chosen as 12 inches in this case as compared to one inch in the previous case, therefore the magnitude of the viscous terms in this mildly viscous case is diminished by a factor of 12 as compared to the previous very viscous case. As expected, the resulting axial wall pressure distribution falls between that of the inviscid and very viscous calculation over the central portion of the nozzle, these results being depicted in Figure (12).

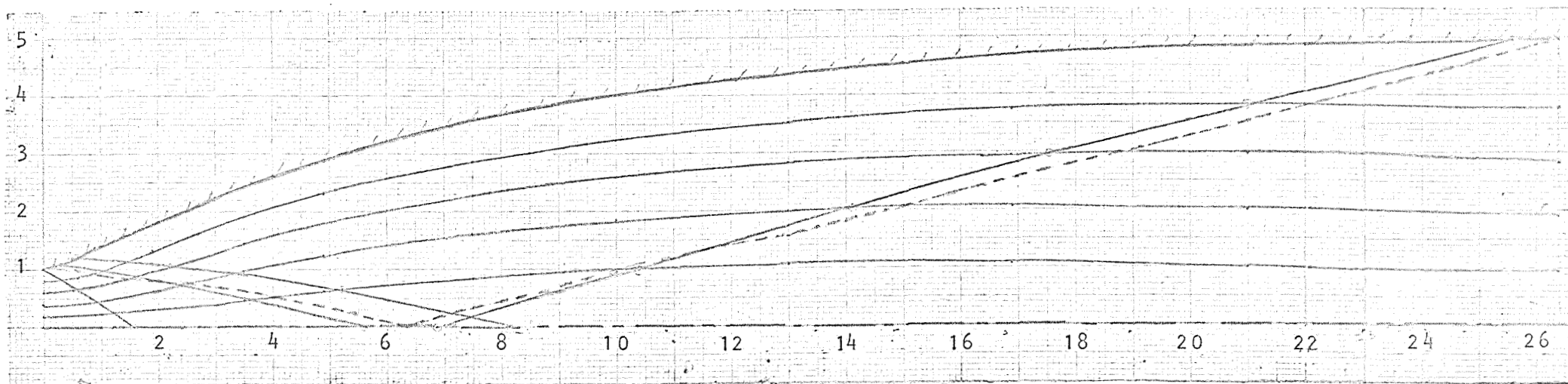


FIGURE 9. DESIGN CONTOUR AND STREAMLINE PATTERN

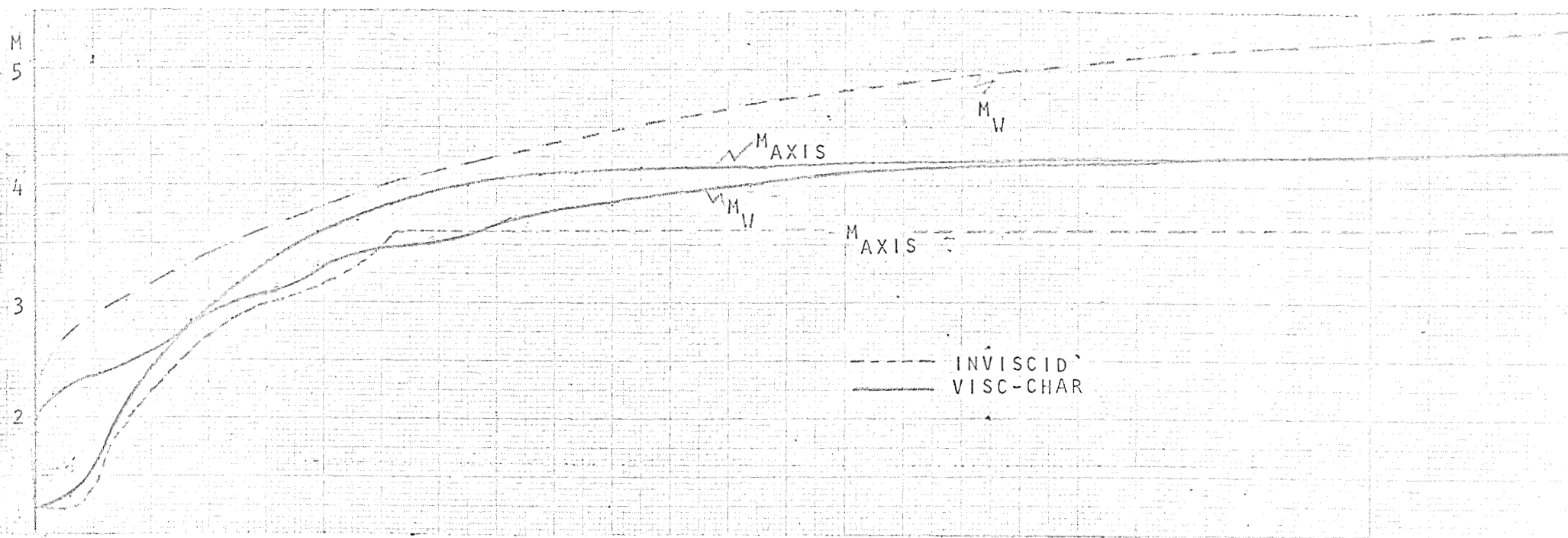


FIGURE 10. AXIAL MACH NUMBER DISTRIBUTIONS

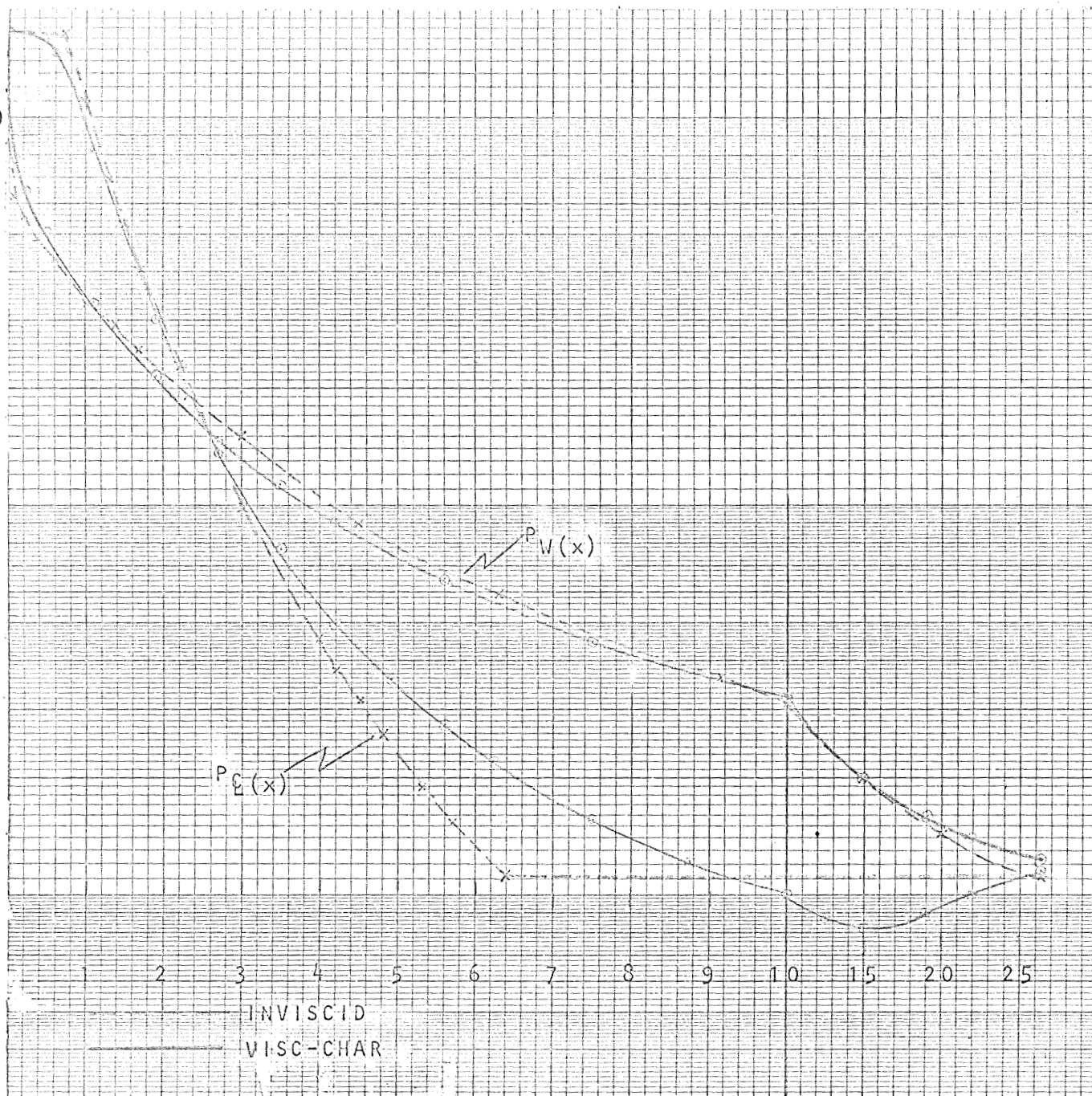


FIGURE 11. AXIAL PRESSURE DISTRIBUTIONS

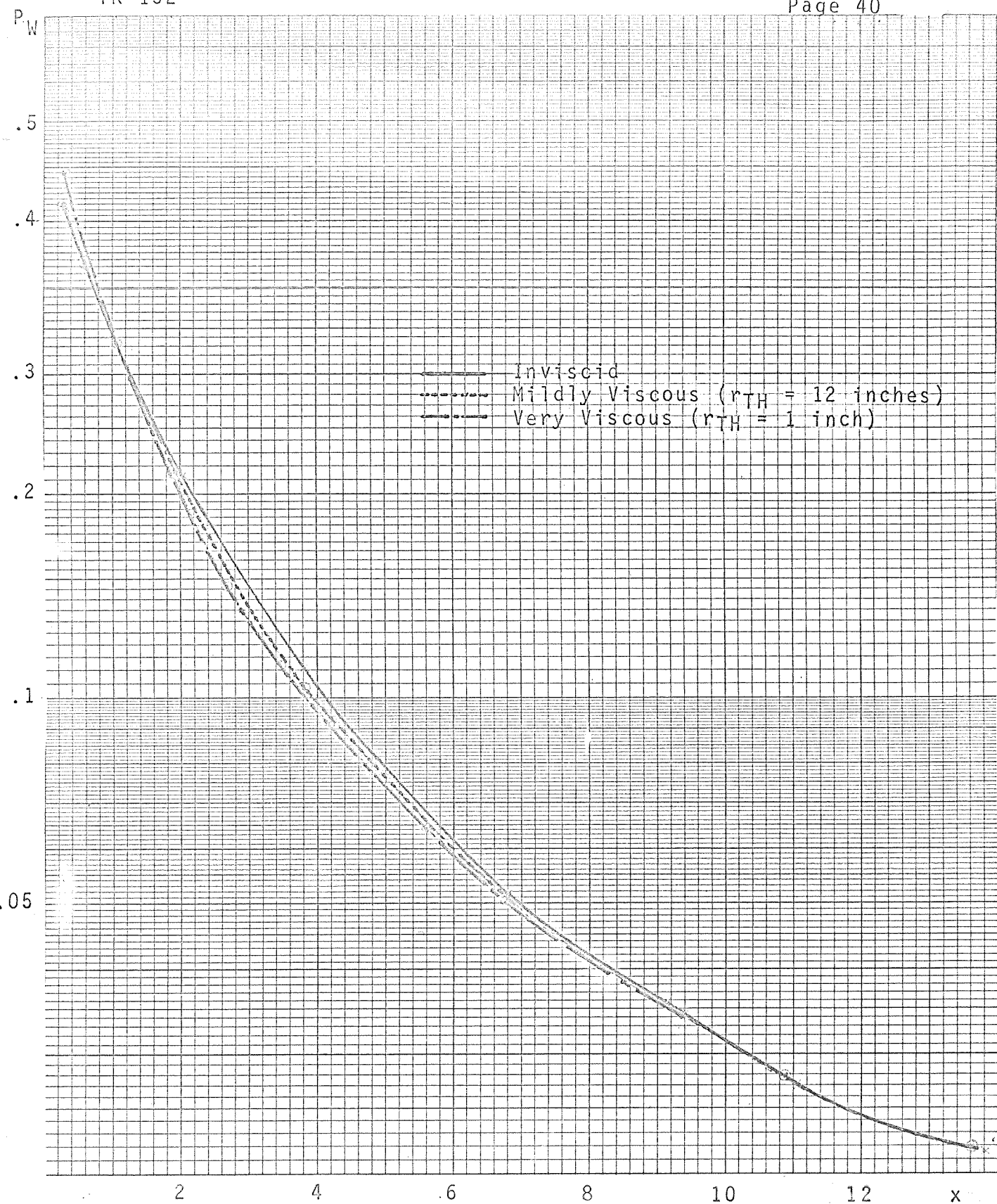


FIGURE 12. AXIAL WALL PRESSURE DISTRIBUTIONS

Thrust computations for the above three cases were performed by integration of the wall pressure distribution, the thrust being computed using Equation (50).

$$\text{Thrust} = (2\pi)^J \int_0^{x_{\text{exit}}} (P - P_\infty) \sin \theta_W (y_W)^J dx \quad (50)$$

The very viscous case ($r_{\text{throat}} = 1$ inch) had approximately a six percent loss in thrust as compared to the inviscid case, while the mildly viscous case had about a four percent loss. These losses are solely due to viscous dissipation resulting from nonuniformities at the nozzle entrance and do not include the effects of skin friction at the nozzle wall.

For a sample calculation with finite rate hydrogen-air chemistry, the same initial profile and nozzle were chosen with H_2 added ($\alpha_{\text{H}_2} = .007$) in the central core. To speed up the occurrence of combustion, small amounts of O , H and OH^* were included in the initial profile, thereby reducing ignition delay time. Pressure and temperature profiles are presented in Figure (13) for both the frozen and finite rate viscous calculations at an axial station just under 2 throat radii downstream of the initial station. The higher temperature

* ($\alpha_{\text{O}} = \alpha_{\text{H}} = \alpha_{\text{OH}} \sim 8 \times 10^{-4}$)

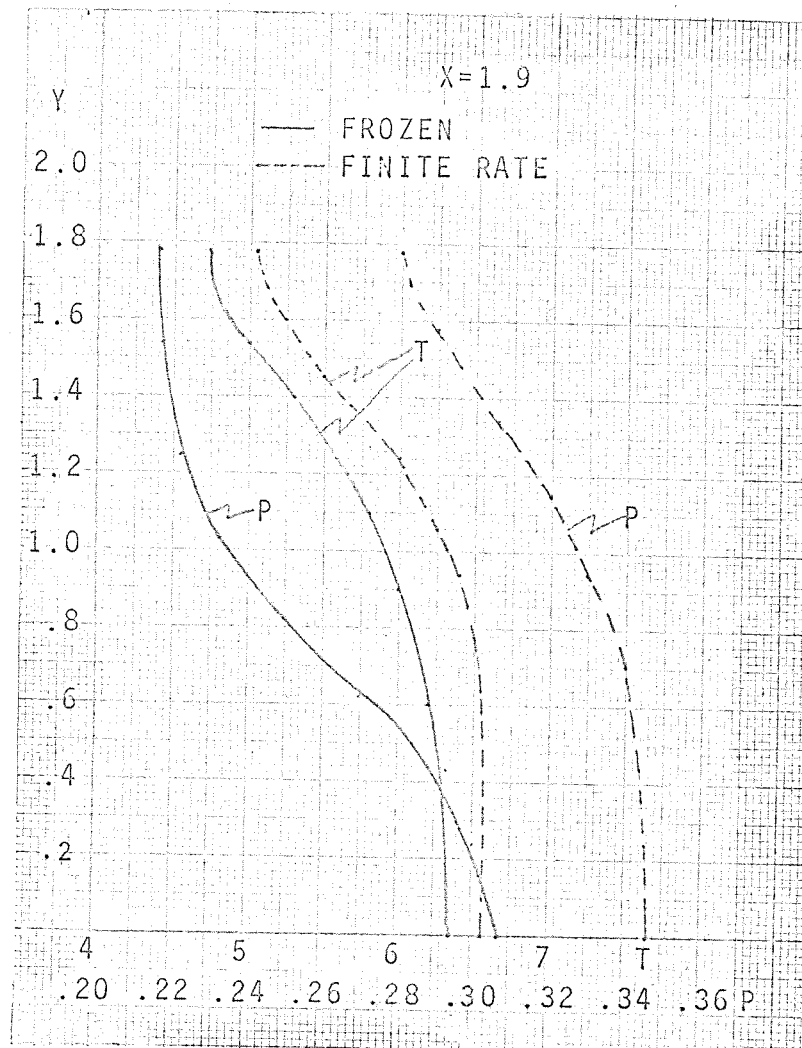


FIGURE 13. RADIAL PRESSURE AND TEMPERATURE DISTRIBUTIONS

profile in the finite rate case reflects the heat generated by the combustion process and the correspondingly higher pressure is a result of the streamline deflections induced by the chemistry.

The axial pressure distributions are presented in Figure (14) for the wall and axis streamlines. Note that at the wall combustion begins almost immediately with a consequent deviation in pressure from the frozen case quite apparent at $x = .1$. Since the chemistry generates a temperature rise at the wall, the Mach number there is lower, hence, signals reach the axis earlier. This is evident in Figure (20) by noting that the axis pressure feels the expansion earlier in the finite rate case. Note that there are two opposing effects; namely, the expansion generated by the wall turning and the compression generated by the chemistry. The wall expansion evidently dominates the overall pressure variation.

The sample calculations performed demonstrate the capability of the viscous-characteristic program to determine internal supersonic flow fields taking into account the effects of shear, conduction and diffusion, as well as finite rate hydrogen-air combustion. The results of these calculations indicate significant differences in thrust between the viscous and inviscid cases, due basically to the large value assumed for the turbu-

lent viscosity, which was chosen to magnify this difference. In using this program for the analysis of an actual nozzle the choice of an appropriate viscosity model must be made by the user, as must the choice in size of the numerical grid, the latter based on a compromise between running time and truncation error.

Regarding the finite rate chemical calculation, the ability of the viscous characteristic program to predict a temperature rise and a corresponding pressure rise induced by chemistry in the presence of a large inviscidly created pressure field, has been demonstrated. It is generally quite difficult to obtain an initial profile and a viscosity model which will simulate actual conditions when finite rate chemistry is involved. The ignition delay time is dependent on both the concentration of radicals (O, H and OH) in the initial profile as well as on the rate of diffusion of H_2 into the air stream. In addition, the size and shape of the combustion zone and accompanying streamline pattern are quite sensitive to the viscosity model employed. For a fixed initial profile, the value of viscosity regulates the amount of fuel diffusing into the combustion zone, as well as the amount of heat conducted away from the flame. The varying pressure across the combustion zone, due to the induced streamline deflections, further complicates the situation, since the chemical rate constants are related

to the pressure level in a non-linear fashion. It is felt that using the viscous characteristics program in conjunction with an experimental program would greatly extend its usefulness and should lead to a greater understanding of the complex interplay between chemistry and mixing in a nonuniform wave field.

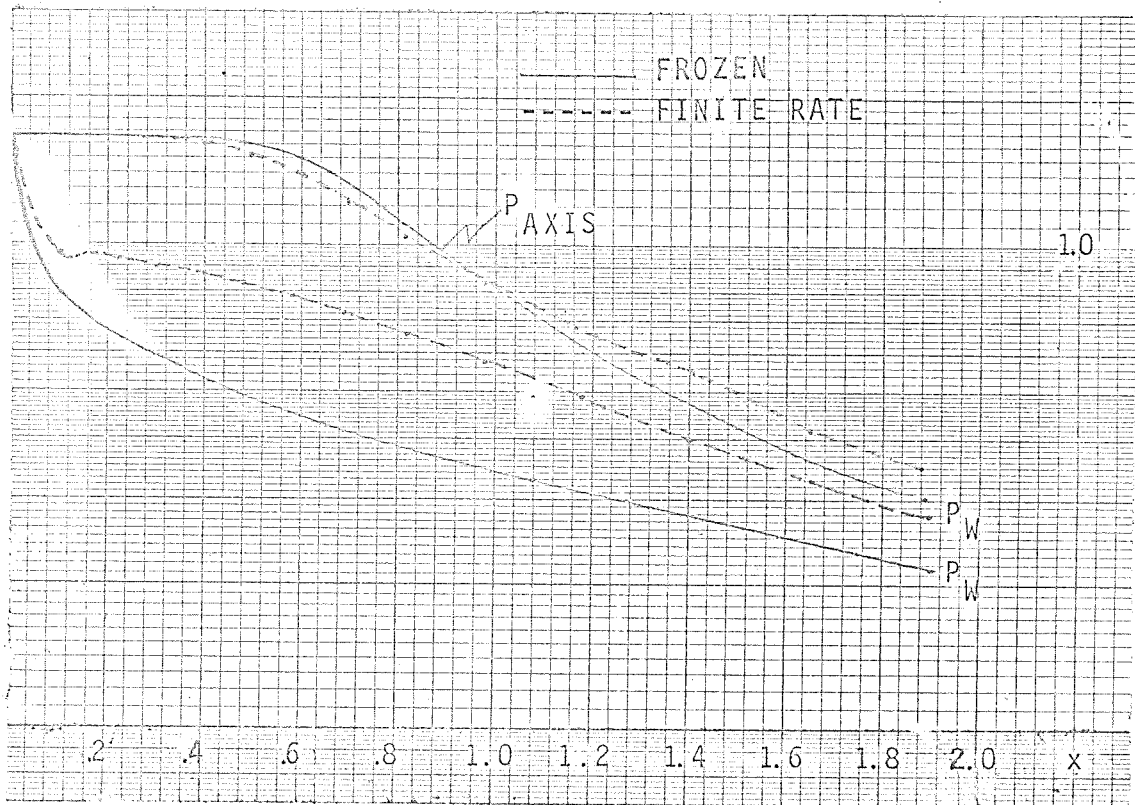


FIGURE 14. STREAMLINE PRESSURE VARIATIONS

APPENDIX-I
CHARACTERISTIC DERIVATION

The continuity equation, expanded, takes the form:

$$\rho \frac{\partial q}{\partial s} + q \frac{\partial \rho}{\partial s} + \rho q \frac{\partial \theta}{\partial n} + \frac{J \rho q}{y} \sin \theta = 0 \quad (I.1)$$

By use of the s-momentum equation, the term $\rho \frac{\partial q}{\partial s}$ may be replaced by

$$\frac{-1}{q} \frac{\partial p}{\partial s} + \frac{S_1}{q} \quad (I.2)$$

Differentiating the equation of state with respect to s yields

$$\frac{\partial \rho}{\partial s} = \frac{W}{W_\infty} \frac{\gamma_\infty M_\infty^2}{T} \frac{\partial p}{\partial s} - W \rho \sum \left(\frac{\frac{\partial \alpha_i}{\partial s}}{m_i} \right) - \frac{\rho}{T} \frac{\partial T}{\partial s} \quad (I.3)$$

where from the conservation of species equation

$$\frac{\frac{\partial \alpha_i}{\partial s}}{m_i} = \frac{1}{\rho q} \left(\frac{S_{3i} + \dot{W}_i}{m_i} \right) \quad (I.4)$$

and from the energy equation

$$\frac{\partial T}{\partial s} = \frac{(\gamma_{\infty}-1)M_{\infty}^2}{\rho q C_p} \left[q \frac{\partial p}{\partial s} + S_2 - \frac{1}{(\gamma_{\infty}-1)M_{\infty}^2} \Sigma \dot{w}_i h_i \right] \quad (I.5)$$

Replacing the terms $\rho \frac{\partial q}{\partial s}$ and $q \frac{\partial \rho}{\partial s}$ appearing in the continuity equation (Equation (I.1)) with the expressions in Equations (I.2) - (I.5), the resulting equation takes the form:

$$\frac{\partial p}{\partial s} \left[\frac{W}{W_{\infty}} \gamma_{\infty} M_{\infty}^2 \frac{q^2}{T} - \frac{(\gamma_{\infty}-1)M_{\infty}^2}{C_p T} q^2 - 1 \right] + \rho q^2 \frac{\partial \theta}{\partial n} = \quad (I.6)$$

$$\frac{-J \rho q^2 \sin \theta}{y} + S_1 + \frac{q(\gamma_{\infty}-1)M_{\infty}^2 S_2}{C_p T} + q W \Sigma \left(\frac{S_{3i} + w_i}{m_i} \right)$$

$$\frac{-q}{C_p T} \Sigma \dot{w}_i h_i$$

By algebraic manipulation, the bracketed term on the left hand side of Equation (I.6) can be reduced to $M_f^2 - 1$. Letting F^* equal the sum of all the terms on the right hand side of Equation (I.6) with the exception of the axisymmetric term $\frac{J \rho q^2 \sin \theta}{y}$, Equation (I.6) takes the form

$$(M_f^2 - 1) \frac{\partial p}{\partial s} + \rho q^2 \frac{\partial \theta}{\partial n} = \frac{-J \rho q^2 \sin \theta}{y} + F^* \quad (I.7)$$

With $\rho q^2 = p M_f^2$, Equation (I.7) and the normal momentum equation are written:

$$\frac{(M_f^2 - 1)}{\gamma p M_f^2} \frac{\partial p}{\partial s} + \frac{\partial \theta}{\partial n} = - \frac{J}{y} \sin \theta + \frac{F^*}{\gamma p M_f^2} \quad (I.8)$$

$$\frac{1}{\gamma p M_f^2} \frac{\partial p}{\partial n} + \frac{\partial \theta}{\partial s} = 0 \quad (I.9)$$

The total derivatives of p and θ may be expressed by:

$$\frac{\partial p}{\partial s} ds + \frac{\partial p}{\partial n} dn = dp \quad (I.10)$$

$$\frac{\partial \theta}{\partial s} ds + \frac{\partial \theta}{\partial n} dn = d\theta \quad (I.11)$$

Written in matrix form, the above system (Equation (I.8) through (I.11)) becomes

$$\begin{pmatrix} (M_f^2 - 1)/\gamma p M_f^2 & 0 & 0 & 1 \\ 0 & 1/\gamma M_f^2 p & 1 & 0 \\ ds & dn & 0 & 0 \\ 0 & 0 & ds & dn \end{pmatrix} \begin{pmatrix} \frac{\partial p}{\partial s} \\ \frac{\partial p}{\partial n} \\ \frac{\partial \theta}{\partial s} \\ \frac{\partial \theta}{\partial n} \end{pmatrix} = \begin{pmatrix} - \frac{J}{y} \sin \theta + \frac{F^*}{\gamma_f p M_f^2} \\ 0 \\ dp \\ d\theta \end{pmatrix} \quad (I.12)$$

The characteristic directions of this system of equations are obtained by setting the determinant of the coefficient matrix equal to zero.

$$\begin{vmatrix} (M_f^2 - 1)/\gamma M_f^2 p & 0 & 0 & 1 \\ 0 & 1/\gamma M_f^2 p & 1 & 0 \\ ds & dn & 0 & 0 \\ 0 & 0 & ds & dn \end{vmatrix} = 0 \quad (I.13)$$

obtaining $\left(\frac{dn}{ds}\right)^2 = \frac{1}{(M_f^2 - 1)}$. Hence the characteristics are lines whose slope is given by

$$\frac{dn}{ds} = \pm \frac{1}{\sqrt{M_f^2 - 1}} = \tan \mu_f \quad (I.14)$$

or expressed in cartesian coordinates

$$\frac{dy}{dx} = \tan (\theta \pm \mu_f) \quad (I.15)$$

The compatibility relation along the characteristics is obtained

by replacing any column of the coefficient matrix with the vector on the right hand side of Equation (I.12) and setting the determinant of this matrix equal to zero.

$$\begin{vmatrix} -\frac{J \sin \theta}{y} + \frac{F^*}{\gamma_{fp} M_f^2} & 0 & 0 & 1 \\ 0 & \frac{1}{\gamma_{fp} M_f^2} & 1 & 0 \\ dp & dn & 0 & 0 \\ d\theta & 0 & ds & dn \end{vmatrix} = 0 \quad (I.16)$$

Expanding the determinant and using Equation (I.14) we obtain the compatibility relation

$$\frac{\sin \mu_f \cos \mu_f}{\gamma_{fp}} dp \pm d\theta + \left[\frac{J \sin \theta}{y} - \frac{F^*}{\gamma_{fp} M_f^2} \right] \frac{\sin \mu_f}{\cos(\theta \pm \mu_f)} dx = 0 \quad (I.17)$$

REFERENCES

1. Ferri, A., "Review of Problems in Application of Supersonic Combustion," Royal Aero. Soc. J., September 1964.
2. Ferri, A., Moretti, G., and Slutsky, S., "Mixing Processes in Supersonic Combustion," J. Soc. Indust. Appl. Math, Vol. 13, No. 1, March 1965.
3. Moretti, G., "Analysis of Two Dimensional Problems of Supersonic Combustion Controlled by Mixing," AIAA Symposium, New York, January 1964.
4. Ferri, A., and Dash, S., "Viscous Flow at High Mach Numbers with Pressure Gradients," Symposium on Viscous Interaction Phenomena in Supersonic and Hypersonic Flow, May 1969.
5. Dash, S., "The Determination of Nozzle Contours for Rotational, Non-Homentropic Gas Mixtures," Advanced Technology Labs., Tech. Rept. No. 148, March 1970
6. Richtmyer, R., and Morton, K., "Difference Methods for Initial Value Problems," Interscience Publishers, New York, 1967
7. McBride, B. J., Heimel, S., Ehlers, J. G., and Gordon, S., "Thermodynamic Properties to 6000°K for 210 Substances Involving the First 18 Elements," NASA SP-3001, 1963.
8. Abett, M. J., "Users Manual for the One Dimensional Fluid Flow, Finite Rate Chemical Kinetics Program with Specified Pressure or Area for the Hydrogen-Air System," General Applied Science Labs., Inc., TR 597, February 1966.
9. Moretti, G., "A New Technique for the Numerical Analysis of Nonequilibrium Flows," AIAA Journal, Vol. 3, No. 2, February 1965, pp. 223-229.
10. Kalben, P., "A Fortran Program for the Determination of Nozzle Contours for Rotational, Non-Homentropic Gas Mixtures," Advanced Technology Labs., Tech. Mem. No. 148, March 1970.