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ERROR ANALYSIS OF THE LINEARIZED METHOD OF CHARACTERISTICS FOR NONEQUILIBRIUM FLOW

J. T. Lee
A. G. Hammitt
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SPACE TECHNOLOGY LABORATORIES, INC.
A SUBSIDIARY OF THOMPSON RAMO WOOLDRIDGE INC.
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ABSTRACT

The pressure on an infinite sinusoidal wall in steady two-dimensional supersonic flow of an inviscid gas in vibrational or chemical nonequilibrium is obtained by the linearized method of characteristics and compared to the analytical solution of the linearized equations previously obtained by Vincenti. The system of "frozen" characteristics is used. At near-equilibrium conditions the error in the method of characteristics is due entirely to the error in integrating the rate equation along the streamlines and can be made arbitrarily small by decreasing the size of the characteristic net. There appears to be no approximate criteria for reducing the error at near-equilibrium conditions by switching over to the system of equilibrium characteristics which are applicable to the entire flow field.

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SYMBOLS

A	parameter defined by Equation (15)
c_p	specific heat at constant pressure
c_i	vibrational heat capacity
D, E	parameters defined by Equations (26) and (27)
h	enthalpy
k	rate parameter defined by Equation (11)
$K_{1, 2, \dots}$	parameters in Taylor series expansion of error terms
l	characteristic dimension of flow field; wavelength of sinusoidal wall
M	Mach number
p	pressure
P	pressure coefficient
q	quantity describing vibrational or chemical state of gas
$\bar{q}$	local equilibrium value of q
R	gas constant
T	temperature
T_i	vibrational temperature
u, v	x, y velocity components
U_∞	free-stream velocity
x	coordinate parallel to wall
y	coordinate normal to wall
Δx	measure of size of characteristic net
$\Delta p, \Delta q', \Delta \bar{q}'$	error terms
$\Delta p^*, \Delta P^*$	maximum difference between equilibrium and frozen pressure along wall

GREEK SYMBOLS

α	Mach angle
δ, λ	parameters defined by Equation (10)
ϵ	amplitude of sinusoidal wall
ρ	density
τ	relaxation time
ϕ	initial value of x for characteristic calculations

SUBSCRIPTS

a	value taken from Vincenti's analytical solution
c	value obtained by method of characteristics
e	equilibrium value
F	frozen value
∞	free-stream conditions
$1, 2, 3$	values at points 1, 2, 3 (see Figure 1)

SUPERSCRIPTS

$'$	perturbation quantity
(n)	value after n iterations
$*$	reference quantity

1. INTRODUCTION

The phenomena of wave propagation and the existence of characteristic surfaces in nonequilibrium flow have been studied by several investigators (e.g., References 1 and 2). It has been well established that characteristics exist for supersonic steady flow and are determined by the frozen speed of sound for all finite values of the reaction rate regardless of how large the reaction rate becomes. When the reaction rate becomes infinite, however, the characteristics are determined by the equilibrium speed of sound. This discontinuous change in the identity of the characteristics is related to a reduction in the order of the governing differential equations for an infinite reaction rate. It has been shown, however, that the analytic solution for a flow field is a continuous function of reaction rate (e.g., References 2 and 3). Thus a near equilibrium solution approaches the usual equilibrium solution as the reaction rate approaches infinity.

If it is desired to set up a calculation procedure based upon the method of characteristics that will be valid for all reaction rates the system of frozen characteristics must be used. Since only finite reaction rates are physically possible anyway, such a procedure would appear to be quite satisfactory. However, the characteristic equations can in general be solved only by use of finite difference methods, and certain errors are therefore introduced. In the usual calculations for perfect or equilibrium gases these errors are known to be dependent on the size of the characteristic net, $\Delta x/l$, where l is a characteristic dimension of the flow field. The introduction of a new dimension into the problem, namely the relaxation length $\tau_{\infty} U_{\infty}$, intuitively suggests that the error will depend also on the parameter $\Delta x/\tau_{\infty} U_{\infty}$.

Practical considerations in calculating a flow field place a certain lower limit on $\Delta x/l$. Thus as the reaction rate becomes large for a fixed value of $\Delta x/l$ the parameter $\Delta x/\tau_{\infty} U_{\infty}$ becomes large and suggests large errors. For near equilibrium flow it seems likely that there is a certain value of the reaction rate above which the error could be reduced by switching over to the system of equilibrium characteristics.

The work described in this report was undertaken in an attempt to provide a better understanding of the errors associated with the calculation of a nonequilibrium flow field by the method of characteristics. In particular, criteria were sought that will predict at what large value of reaction rate the equilibrium characteristics should be used. The analytic solution obtained by Vincenti, Reference 3, for the linearized nonequilibrium flow past an infinite sinusoidal wall was compared with results obtained by the method of characteristics solution of the same linearized flow equations. Vincenti's analytic solution has the advantage of being relatively simple so that the algebra involved is not prohibitive. The linearized equations offer another advantage in that for frozen flow the solution obtained by the method of characteristics is exact for all net size. All errors can therefore be attributed directly to the nonequilibrium aspects of the flow.

2. LINEARIZED EQUATIONS AND SOLUTION FOR A WAVY WALL

The linearized equations of motion for a gas subject to a single relaxation process were derived by Vincenti in Reference 3. It was assumed that the flow field is described by a perturbation of a uniform parallel flow with velocity U_∞ in the x direction such that $u = U_\infty + u'$, $v = v'$, $p = p_\infty + p'$, etc. It was also assumed that the uniform flow is in equilibrium. The resulting equations are:

Continuity:

$$\rho_\infty \left(\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} \right) + U_\infty \frac{\partial \rho'}{\partial x} = 0 \quad (1)$$

x Momentum:

$$\rho_\infty U_\infty \frac{\partial u'}{\partial x} + \frac{\partial p'}{\partial x} = 0 \quad (2)$$

y Momentum:

$$\rho_\infty U_\infty \frac{\partial v'}{\partial x} + \frac{\partial p'}{\partial y} = 0 \quad (3)$$

Energy:

$$U_\infty \frac{\partial u'}{\partial x} + \frac{\partial h'}{\partial x} = 0 \quad (4)$$

Equation of State:

$$dh' = \left(\frac{\partial h}{\partial p} \right)_\infty dp' + \left(\frac{\partial h}{\partial \rho} \right)_\infty d\rho' + \left(\frac{\partial h}{\partial q} \right)_\infty dq' \quad (5)$$

Rate Equation:

$$\frac{\partial q'}{\partial x} = \frac{\bar{q}' - q'}{\tau_\infty U_\infty} \quad (6)$$

Equilibrium Relation:

$$d\bar{q}' = \left(\frac{\partial \bar{q}}{\partial p} \right)_\infty dp' + \left(\frac{\partial \bar{q}}{\partial \rho} \right)_\infty d\rho' \quad (7)$$

The coordinate system used is shown in Figure 1.

The quantity q describes the vibrational or chemical state of the gas. For vibrational relaxation q is the vibrational temperature, and for chemical relaxation q is the dissociation mass fraction. The quantity $\bar{q}$ is a fictitious local equilibrium value of q determined by the nonequilibrium values of p and ρ .

Vincenti analyzed the flow past an infinite sinusoidal wall by introducing a velocity potential and solving the resulting third order linear potential equation. Details of the method and results are contained in Reference 3. The perturbation velocities are:

$$\frac{u'}{U_\infty} = \frac{2\pi \frac{\epsilon}{l}}{\delta^2 + \lambda^2} e^{-2\pi\delta \frac{y}{l}} \left(\delta \sin 2\pi \frac{x - \lambda y}{l} - \lambda \cos 2\pi \frac{x - \lambda y}{l} \right) \quad (8)$$

$$\frac{v'}{U_\infty} = 2\pi \frac{\epsilon}{l} e^{-2\pi\delta \frac{y}{l}} \cos 2\pi \frac{x - \lambda y}{l} \quad (9)$$

The parameters δ and λ are given by

$$\left\{ \frac{\delta}{\lambda} \right\} = \left(\frac{1}{2(1+k^2)} \left\{ \pm \left(1 - M_{e\infty}^2 \right) \pm k^2 \left(1 - M_{F\infty}^2 \right) + \sqrt{(1+k^2) \left[\left(1 - M_{e\infty}^2 \right)^2 + k^2 \left(1 - M_{F\infty}^2 \right)^2 \right]} \right\} \right)^{\frac{1}{2}} \quad (10)$$

where

$$k = \left(\frac{\frac{\partial h}{\partial \rho}}{\frac{\partial h}{\partial \rho} + \frac{\partial h}{\partial q} \frac{\partial \bar{q}}{\partial \rho}} \right)_\infty 2\pi \frac{\tau_\infty U_\infty}{l} \quad (11)$$

Disturbances in the flow field are propagated along the lines $(dy/dx) = 1/\lambda$, and δ is a measure of the rate of decay of these disturbances. In the equilibrium and frozen limit for supersonic flow these parameters become:

	<u>Equilibrium</u>	<u>Frozen</u>
δ	0	0
λ	$\sqrt{M_{e\infty}^2 - 1}$	$\sqrt{M_{F\infty}^2 - 1}$

(12)

3. SOLUTION BY METHOD OF CHARACTERISTICS

The characteristic relations for the linearized Equations (1) through (7) were obtained by the usual method of solving for a particular derivative, such as $\partial u'/\partial x$ and setting the determinants in the numerator and denominator equal to zero. For all finite reaction rates, $0 \leq t/\tau_\infty U_\infty < \infty$, the characteristics are:

along

$$\left. \begin{aligned} \frac{dy}{dx} &= \pm \tan \alpha_F \\ dp' \pm \rho_\infty U_\infty \tan \alpha_F dv' - A \frac{\bar{q}' - q'}{\tau_\infty U_\infty} dx &= 0 \end{aligned} \right\} \quad (13)$$

along

$$\left. \begin{aligned} \frac{dy}{dx} &= 0 \\ \frac{dq'}{dx} &= \frac{\bar{q}' - q'}{\tau_\infty U_\infty} \end{aligned} \right\} \quad (14)$$

where

$$A = \frac{\tan^2 \alpha_F U_\infty^2 \left(\frac{\partial h}{\partial q} \right)_\infty}{\left(\frac{\partial h}{\partial p} \right)_\infty} \quad (15)$$

$$\alpha_F = \tan^{-1} \frac{1}{\sqrt{M_{F_\infty}^2 - 1}} \quad (16)$$

Thus the characteristic direction is determined by the frozen speed of sound for all finite reaction rates. In the linearized approximation the lines $(dy/dx) = 0$ are streamlines and Equation (14) is just the rate equation following a fluid particle.

For flow that is everywhere identically in equilibrium, $l/\tau_\infty U_\infty \equiv \infty$, the characteristic relations can be obtained by substituting $\bar{q} \equiv q'$ into Equations (1) through (7) and proceeding as before. The results are:

along

$$\begin{aligned} \frac{dy}{dx} &= \pm \tan \alpha_e \\ dp' \pm \rho_\infty U_\infty \tan \alpha_e dv' &= 0 \end{aligned} \quad (17)$$

where

$$\alpha_e = \tan^{-1} \frac{1}{\sqrt{M_{e\infty}^2 - 1}} \quad (18)$$

The discontinuous change from the frozen to the equilibrium characteristics as $l/\tau_\infty U_\infty \rightarrow \infty$ brings up the question of what errors are introduced in calculating near equilibrium flow using the frozen characteristics. In equilibrium gas calculations the error which results from solving the characteristic equations by finite difference methods is known to depend on the size of the characteristic net, $\Delta x/l$. The introduction of a new characteristic length into the problem (i. e., the relaxation length, $\tau_\infty U_\infty$) suggests that the error will now depend also on the parameter $\Delta x/\tau_\infty U_\infty$.

To study this error, the pressure at a wall point as calculated by the method of characteristics, p_c , is compared to Vincenti's analytic solution, p_a . A convenient parameter for expressing the error is defined as:

$$\frac{\Delta p}{\Delta p^*} = \frac{(p_3)_c - (p_3)_a}{(p_e - p_F)_{\text{max along wall}}} \quad (19)$$

where p_3 is the pressure at the wall point 3 (see Figure 1). This parameter is calculated as a function of net size, $\Delta x/l$, and reaction rate, $l/\tau_\infty U_\infty$. All quantities along the vertical line $x = \phi$ and the reference pressure Δp^* are taken from the analytic solution, and Δp^* is given by:

$$\Delta p^* = 2\pi \rho_\infty U_\infty^2 \frac{\epsilon}{l} (\tan \alpha_F - \tan \alpha_e) \quad (20)$$

Applying Equation (13) in finite difference form along the characteristic 1-3 gives:

$$p_3' = p_1' + \rho_\infty U_\infty \tan \alpha_F (v_3' - v_1') + \frac{A}{2} [(\bar{q}_1' - q_1') + (\bar{q}_3' - q_3')] \frac{\Delta x}{\tau_\infty U_\infty} \quad (21)$$

The term $\bar{q}_3'$ can be eliminated by noting that:

$$\bar{q}_3' = \bar{q}_1' + (\bar{q}_3' - \bar{q}_1') \quad (22)$$

The differential form of Equations (2) and (4) can be written as:

$$\rho_\infty U_\infty du' + dp' = 0 \quad (23)$$

$$U_\infty du' + dh' = 0 \quad (24)$$

Equations (23) and (24) can be combined with (5) and (7) to give:

$$d\bar{q}' = Ddp' + Edq' \quad (25)$$

where

$$D = \left[\frac{\partial \bar{q}}{\partial p} + \frac{\frac{\partial \bar{q}}{\partial \rho}}{\rho \frac{\partial h}{\partial \rho}} - \frac{\frac{\partial \bar{q}}{\partial \rho} \frac{\partial h}{\partial p}}{\frac{\partial h}{\partial \rho}} \right]_\infty \quad (26)$$

$$E = - \left[\frac{\frac{\partial \bar{q}}{\partial \rho} \frac{\partial h}{\partial q}}{\frac{\partial h}{\partial \rho}} \right]_\infty \quad (27)$$

Equation (22) can now be written as:

$$\bar{q}_3' = \bar{q}_1' + D(p_3' - p_1') + E(q_3' - q_1') \quad (28)$$

To obtain the pressure at 3 from Equations (21) and (28), the rate equation [Equation (14)] must be integrated along the wall streamline from 2 to 3 to obtain q_3' . It is convenient and instructive to assume that this integration introduces an error $\Delta q'$ in q_3' defined by:

$$q_3' = (q_3')_a + \Delta q' \quad (29)$$

Substituting Equations (28) and (29) into (21) gives the error in pressure as:

$$\frac{\Delta p}{\Delta p^*} = \left\{ \frac{p_1' + \rho_\infty U_\infty \tan \alpha_F (v_3' - v_1') + \frac{A}{2} [2\bar{q}_1' - q_1' - Dp_1' - Eq_1' + (E-1)(q_3')_a] \frac{\Delta x}{\tau_\infty U_\infty}}{\Delta p^* \left(1 - \frac{AD}{2} \frac{\Delta x}{\tau_\infty U_\infty}\right)} - \frac{(p_3')_a}{\Delta p^*} \right\} + \frac{\frac{A}{2} (E-1) \frac{\Delta x}{\tau_\infty U_\infty}}{1 - \frac{DA}{2} \frac{\Delta x}{\tau_\infty U_\infty}} \frac{\Delta q_1'}{\Delta p^*} \quad (30)$$

where v_3' can be evaluated using the linearized boundary condition at the wall:

$$(v')_{\text{wall}} = 2\pi U_\infty \frac{\epsilon}{l} \cos 2\pi \frac{x}{l} \quad (31)$$

Thus the error consists of two distinct parts. The term in $\{ \}$ in Equation (30) is the error which results from the averaging of quantities in the finite difference relation along the inclined characteristic 1-3. The remaining term in Equation (30) is the error in pressure associated with the error in integrating the rate equation along the streamline 2-3. We denote these in errors I and II respectively so that:

$$\frac{\Delta p}{\Delta p^*} = \left(\frac{\Delta p}{\Delta p^*} \right)_I + \left(\frac{\Delta p}{\Delta p^*} \right)_{II} \quad (32)$$

Vincenti's analytic solution is used to evaluate the term $(\Delta p / \Delta p^*)_I$. The resulting complicated expression can be simplified by expanding it in a Taylor series about $\Delta x / l = 0$ giving:

$$\left(\frac{\Delta p}{\Delta p^*} \right)_I = \frac{K_1 \left(\frac{\Delta x}{l} \right)^3 + K_2 \left(\frac{\Delta x}{l} \right)^4 + \dots}{1 + K_4 \left(\frac{\Delta x}{l} \right)} \quad (33)$$

where

$$K_4 = - \frac{AD}{2} \frac{l}{\tau_\infty U_\infty} \quad (34)$$

The parameters K_1 and K_2 were determined for two values of ϕ :

at $\phi = 0$:

$$K_1 = \frac{2\pi^3 \tan^2 \alpha_F \delta}{3(\tan \alpha_F - \tan \alpha_e)} \left\{ 3(\lambda \tan \alpha_F)^2 + 4\lambda \tan \alpha_F + \frac{1}{(\lambda \tan \alpha_F)^2} \right\} \quad (35)$$

$$K_2 = \frac{2\pi^4 \tan \alpha_F}{3(\tan \alpha_F - \tan \alpha_e)} \left\{ (\lambda \tan \alpha_F)^4 + (\lambda \tan \alpha_F)^3 - 2(\lambda \tan \alpha_F)^2 - 2\lambda \tan \alpha_F + 1 + (\lambda \tan \alpha_F)^{-1} \right\} \quad (36)$$

at $\phi = 1/4$:

$$K_1 = \frac{2\pi^3}{3\lambda(\tan \alpha_F - \tan \alpha_e)} \left\{ -(\lambda \tan \alpha_F)^4 - 2(\lambda \tan \alpha_F)^3 \frac{\lambda^2}{\delta^2 + \lambda^2} + \frac{\lambda^2}{\delta^2 + \lambda^2} + 2\lambda \tan \alpha_F \right\} \quad (37)$$

$$K_2 = \frac{2\pi^4 \delta}{3\lambda^2(\tan \alpha_F - \tan \alpha_e)} \left\{ 4(\lambda \tan \alpha_F)^5 + 3(\lambda \tan \alpha_F)^4 \frac{\lambda^2}{\delta^2 + \lambda^2} - 4(\lambda \tan \alpha_F)^3 - 2(\lambda \tan \alpha_F)^2 - \frac{\lambda^2}{\delta^2 + \lambda^2} \right\} \quad (38)$$

In both the equilibrium and frozen limit the quantity $(\Delta p / \Delta p^*)_I$ goes to zero. The error in calculating the pressure by the linearized method of characteristics for near equilibrium flow is therefore due entirely to the error in integrating the rate equation along the streamline.

In evaluating the term $(\Delta p / \Delta p^*)_{II}$ it is convenient to introduce the pressure coefficient,

$$P = \frac{p - p_\infty}{1/2 \rho_\infty U_\infty^2}$$

such that:

$$\left(\frac{\Delta p}{\Delta p^*}\right)_{II} = \frac{K_9 \frac{\Delta x}{l}}{1 + K_4 \frac{\Delta x}{l}} \left(\frac{\Delta q'}{T_\infty \Delta P^*}\right) \quad (39)$$

where:

$$K_9 = A(E - 1) \frac{T_\infty}{\rho_\infty U_\infty^2} \frac{l}{\tau_\infty U_\infty} \quad (40)$$

A first approximation for q_3' is:

$$q_3'^{(1)} = q_2' + \left(\frac{dq'}{dx}\right)_2 \Delta x \quad (41)$$

The error in $q_3'^{(1)}$ can be found by expanding $q'(x)$ in a Taylor series about $\Delta x = 0$:

$$(q_3')_a = q_2' + \left(\frac{dq'}{dx}\right)_2 \Delta x + \frac{1}{2} \left(\frac{d^2 q'}{dx^2}\right)_2 \Delta x^2 + \frac{1}{6} \left(\frac{d^3 q'}{dx^3}\right)_2 \Delta x^3 + \dots \quad (42)$$

Subtracting Equation (42) from (41) gives:

$$\Delta q'^{(1)} = -\frac{1}{2} \left(\frac{d^2 q'}{dx^2}\right)_2 \Delta x^2 - \frac{1}{6} \left(\frac{d^3 q'}{dx^3}\right)_2 \Delta x^3 - \frac{1}{12} \left(\frac{d^4 q'}{dx^4}\right)_2 \Delta x^4 - \dots \quad (43)$$

The derivatives in Equation (43) are evaluated using Vincenti's solution at $x = \phi$. This results in:

$$\frac{\Delta q'^{(1)}}{T_\infty \Delta P^*} = K_7 \left(\frac{\Delta x}{l}\right)^2 - 2K_8 \left(\frac{\Delta x}{l}\right)^3 - \frac{\pi^2}{3} K_7 \left(\frac{\Delta x}{l}\right)^4 + \dots \quad (44)$$

where:

at $\phi = 0$:

$$K_7 = \frac{\pi^2 \left(\frac{\partial h}{\partial \rho} \right)_{\infty} \left(\lambda \tan^2 \alpha_F - \frac{\lambda}{\delta^2 + \lambda^2} \right)}{\left(\frac{\partial h}{\partial q} \right)_{\infty} \left(\frac{\partial \bar{q}}{\partial \rho} \right)_{\infty} \tan^2 \alpha_F (\tan \alpha_F - \tan \alpha_e)} \quad (45)$$

$$K_8 = - \frac{\pi^3 \left(\frac{\partial h}{\partial \rho} \right)_{\infty} \left(\delta \tan^2 \alpha_F + \frac{\delta}{\delta^2 + \lambda^2} \right)}{\left(\frac{\partial h}{\partial q} \right)_{\infty} \left(\frac{\partial \bar{q}}{\partial \rho} \right)_{\infty} \tan^2 \alpha_F (\tan \alpha_F - \tan \alpha_e)} \quad (46)$$

at $\phi = 1/4$:

$$K_7 = \frac{\pi^2 \left(\frac{\partial h}{\partial \rho} \right)_{\infty} \left(\delta \tan^2 \alpha_F + \frac{\delta}{\delta^2 + \lambda^2} \right)}{\left(\frac{\partial h}{\partial q} \right)_{\infty} \left(\frac{\partial \bar{q}}{\partial \rho} \right)_{\infty} \tan^2 \alpha_F (\tan \alpha_F - \tan \alpha_e)} \quad (47)$$

$$K_8 = \frac{\pi^3 \left(\frac{\partial h}{\partial \rho} \right)_{\infty} \left(\lambda \tan^2 \alpha_F - \frac{\lambda}{\delta^2 + \lambda^2} \right)}{\left(\frac{\partial h}{\partial q} \right)_{\infty} \left(\frac{\partial \bar{q}}{\partial \rho} \right)_{\infty} \tan^2 \alpha_F (\tan \alpha_F - \tan \alpha_e)} \quad (48)$$

The error in q_3' resulting from integration of the rate equation along the streamline can be reduced by use of an iterative procedure as follows:

$$q_3'^{(2)} = q_2' + \frac{1}{2} \left[\left(\frac{dq'}{dx} \right)_2 + \left(\frac{dq'}{dx} \right)_3^{(1)} \right] \Delta x \quad (49)$$

$$\vdots$$

$$q_3'^{(n)} = q_2' + \frac{1}{2} \left[\left(\frac{dq'}{dx} \right)_2 + \left(\frac{dq'}{dx} \right)_3^{(n-1)} \right] \Delta x \quad (50)$$

To obtain the error in $q_3'^{(n)}$ we rewrite Equation (42) as:

$$(q_3')_a = q_2' + \frac{1}{2} \left(\frac{dq'}{dx} \right)_2 \Delta x + \frac{1}{2} \left[\left(\frac{dq'}{dx} \right)_2 + \left(\frac{d^2 q'}{dx^2} \right)_2 \Delta x \right] \Delta x + \frac{1}{6} \left(\frac{d^3 q'}{dx^3} \right)_2 \Delta x^3 + \dots \quad (51)$$

and expand dq'/dx in a Taylor series about $\Delta x = 0$:

$$\left(\frac{dq'}{dx}\right)_{3_a} = \left[\left(\frac{dq'}{dx}\right)_2 + \left(\frac{d^2q'}{dx^2}\right)_2 \Delta x\right] + \frac{1}{2} \left(\frac{d^3q'}{dx^3}\right)_2 \Delta x^2 + \dots \quad (52)$$

Solving Equation (52) for the quantity in [] and substituting this into Equation (51) gives:

$$(q_3')_a = q_2' + \frac{1}{2} \left(\frac{dq'}{dx}\right)_2 \Delta x + \frac{1}{2} \left(\frac{dq'}{dx}\right)_{3_a} \Delta x - \frac{1}{12} \left(\frac{d^3q'}{dx^3}\right)_2 \Delta x^3 + \dots \quad (53)$$

Subtracting Equation (53) from (50) gives:

$$\Delta q^{(n)} = \frac{1}{2} \left[\left(\frac{dq'}{dx}\right)^{(n-1)} - \left(\frac{dq'}{dx}\right)_{3_a} \right] \Delta x + \frac{1}{12} \left(\frac{d^3q'}{dx^3}\right)_2 \Delta x^3 + \dots \quad (54)$$

The rate equation, Equation (14), can be used to express Equation (54) in terms of the errors in $\bar{q}'$ and q' resulting in:

$$\Delta q^{(n)} = \frac{1}{2} \frac{\Delta x}{\tau_\infty U_\infty} \left[\Delta \bar{q}^{(n-1)} - \Delta q^{(n-1)} \right] + \frac{1}{12} \left(\frac{d^3q'}{dx^3}\right)_2 \Delta x^3 + \dots \quad (55)$$

The error in $\bar{q}'$ after $(n-1)$ iterations is obtained from Equation (25):

$$\Delta \bar{q}^{(n-1)} = D \Delta p^{(n-1)} + E \Delta q^{(n-1)} \quad (56)$$

Substituting Equation (56) into (55) and using the parameters introduced in Equation (44) for $(d^3q'/dx^3)_2$ and $(d^4q'/dx^4)_2$ gives:

$$\frac{\Delta q^{(n)}}{T_\infty \Delta P^*} = K_5 \left(\frac{\Delta x}{l}\right) \left(\frac{\Delta p}{\Delta p^*}\right)^{(n-1)} + K_6 \left(\frac{\Delta x}{l}\right) \frac{\Delta q^{(n-1)}}{T_\infty \Delta P^*} + K_8 \left(\frac{\Delta x}{l}\right)^3 + \frac{\pi^2}{3} K_7 \left(\frac{\Delta x}{l}\right)^4 + \dots \quad (57)$$

where:

$$K_5 = \frac{D \rho_\infty U_\infty^2}{4 T_\infty} \frac{l}{\tau_\infty U_\infty} \quad (58)$$

$$K_6 = \frac{1}{2} (E - 1) \frac{l}{\tau_{\infty} U_{\infty}} \quad (59)$$

Equation (57) can now be used with Equations (39) and (44) to find $(\Delta p / \Delta p^*)_{II}$ after an arbitrary number of iterations. The total error in pressure after each iteration, $(\Delta p / \Delta p^*)^{(n)}$, is given by:

$$\left(\frac{\Delta p}{\Delta p^*} \right)^{(n)} = \left(\frac{\Delta p}{\Delta p^*} \right)_I + \left(\frac{\Delta p}{\Delta p^*} \right)_{II}^{(n)} \quad (60)$$

4. NUMERICAL RESULTS AND CONCLUSIONS

The results of Section 3 are applicable to a gas in which either vibrational or chemical relaxation occurs. Numerical values of the error parameter were calculated for a diatomic gas subject to vibrational relaxation for which q is taken to be the vibrational temperature, T_i . The equation of state and the enthalpy are given by;

$$p = \rho R T \quad (61)$$

$$h = c_p T + \int c_i d T_i \quad (62)$$

where c_i is the vibrational heat capacity. The parameters in Section 3 become:

$$K_4 = \frac{1}{5} \tan^2 \alpha_F \frac{c_{i\infty}}{c_p} M_{F\infty}^2 \frac{l}{\tau_{\infty} U_{\infty}} \quad (63)$$

$$K_5 = \frac{1}{10} M_{F\infty}^2 \frac{l}{\tau_{\infty} U_{\infty}} \quad (64)$$

$$K_6 = -\frac{1}{2} \left(1 + \frac{c_{i\infty}}{c_p} \right) \frac{l}{\tau_{\infty} U_{\infty}} \quad (65)$$

where $c_{i\infty}$ is $c_i(T_i)$ evaluated at the free-stream equilibrium temperature, T_{∞} . Results are shown in Figures 2 and 3 with initial conditions taken along $\phi = 0$ and $\phi = l/4$ for various numbers of iterations. The limit error curves obtained after a large number of iterations are replotted in Figure 4 for comparison.

The calculation procedure using the frozen characteristics is seen to be convergent even in the limit of equilibrium flow. The error converges to a limit error curve after a number of iterations and approaches zero with decreasing net size. Since all errors are of order $(\Delta x/l)^2$ or higher, the error in calculating a flow field for all values of $l/\tau_{\infty} U_{\infty}$ and n can be made arbitrarily small by decreasing the size of the characteristic net.

It is noted that for $l/\tau_{\infty} U_{\infty} \rightarrow \infty$ only a single iteration is required to reach the limit error curve. This can be explained by recalling that in the equilibrium limit no error is introduced in the calculation along the inclined characteristic 1-3, i. e.

$$\lim_{\frac{l}{\tau_{\infty} U_{\infty}} \rightarrow \infty} \left(\frac{\Delta p}{\Delta p^*} \right)_I = 0$$

Thus the equilibrium limit of Equation (30) after $(n - 1)$ iterations is:

$$\lim_{\frac{l}{\tau_{\infty} U_{\infty}} \rightarrow \infty} \Delta p^{(n-1)} = - \frac{1}{D} (E - 1) \Delta q^{(n-1)} \quad (66)$$

Substituting Equation (66) into (56) gives:

$$\Delta \bar{q}^{(n-1)} \rightarrow \Delta q^{(n-1)} \text{ as } \frac{l}{\tau_{\infty} U_{\infty}} \rightarrow \infty \quad (67)$$

From Equations (55) and (67) we see that, in the equilibrium limit, $\Delta q^{(n)}$ [and therefore $\Delta p^{(n)}$] is independent of the number of iterations for $n \geq 2$. This behavior is a property of the linearized characteristics and cannot be expected to be valid for the general method of characteristics.

In Figure 2, it is noted that increasing $c_{i\infty}/c_p$ (i. e., increasing the energy associated with the relaxation phenomena) results in a decrease in $\Delta p/\Delta p^*$. Thus the effects of relaxation on the wall pressure distribution increase faster with temperature than the error introduced by the finite difference method of calculating these effects.

If the equilibrium characteristics, Equation (17), were used to calculate p_3 as $l/\tau_{\infty} U_{\infty} \rightarrow \infty$ the error would be identically zero for all net size. Thus there is some large value of $l/\tau_{\infty} U_{\infty}$ at which, for a given net size, it would be better to calculate the flow field using the equilibrium characteristics. In Figure 4, however, it is seen that near equilibrium the error is strongly dependent on the location of the initial line ϕ . Thus

due to the dependence of the error on the gradients of the thermodynamic properties in the flow field. Thus the parameters $\Delta x/l$ and $l/\tau_{\infty} U_{\infty}$ are not sufficient to establish even approximate criteria for switching over to the equilibrium characteristics as $l/\tau_{\infty} U_{\infty}$ becomes large.

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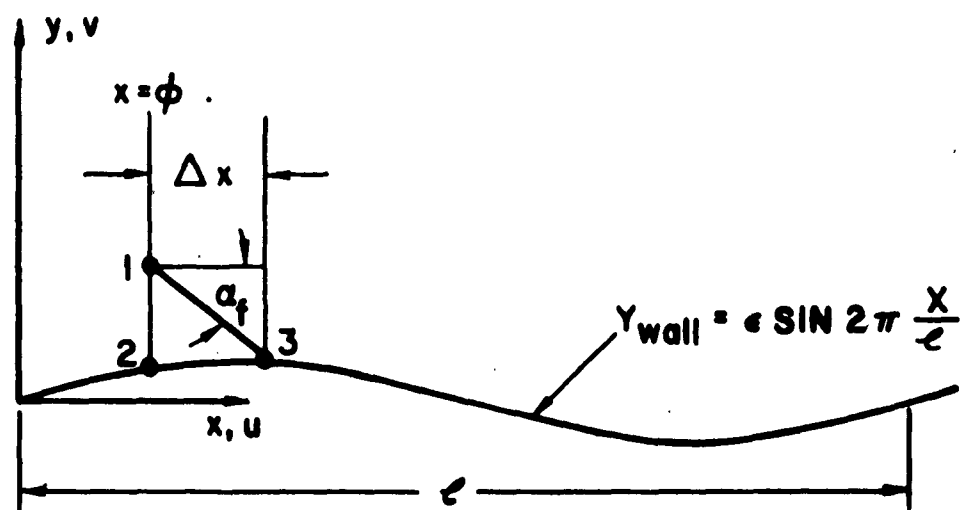


Figure 1. Coordinate System

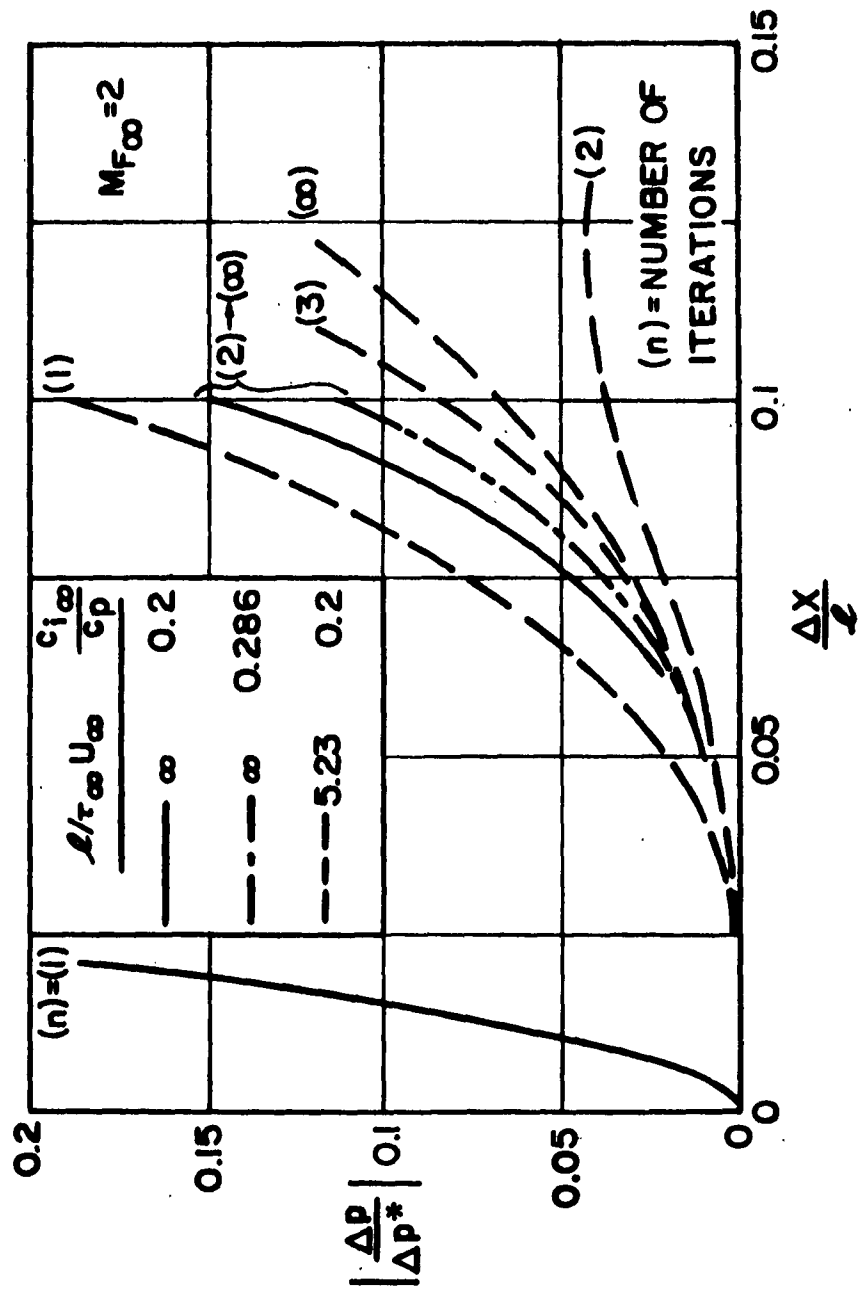


Figure 2. Error in Pressure, $\phi = 0$

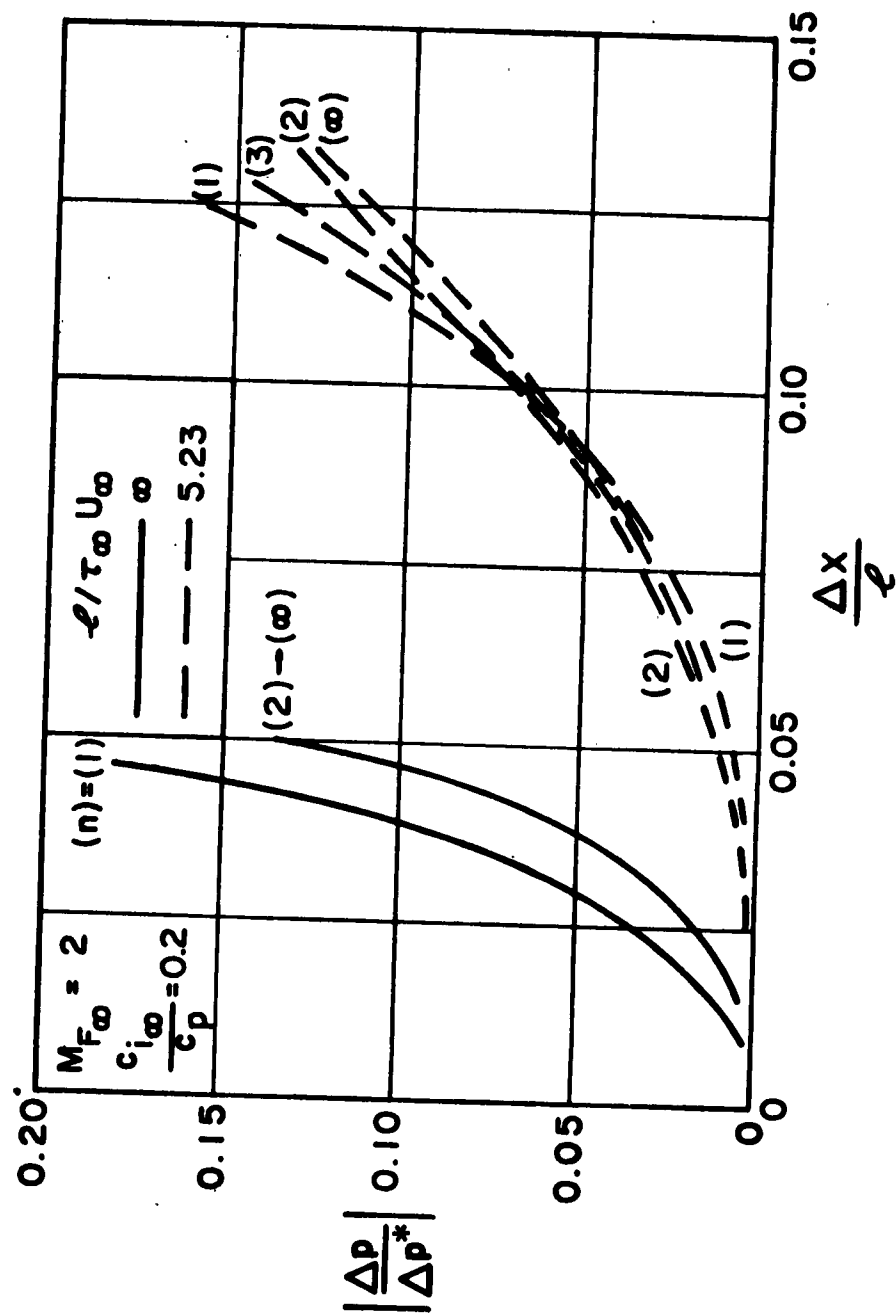


Figure 3. Error in Pressure, $\phi = 1/4$

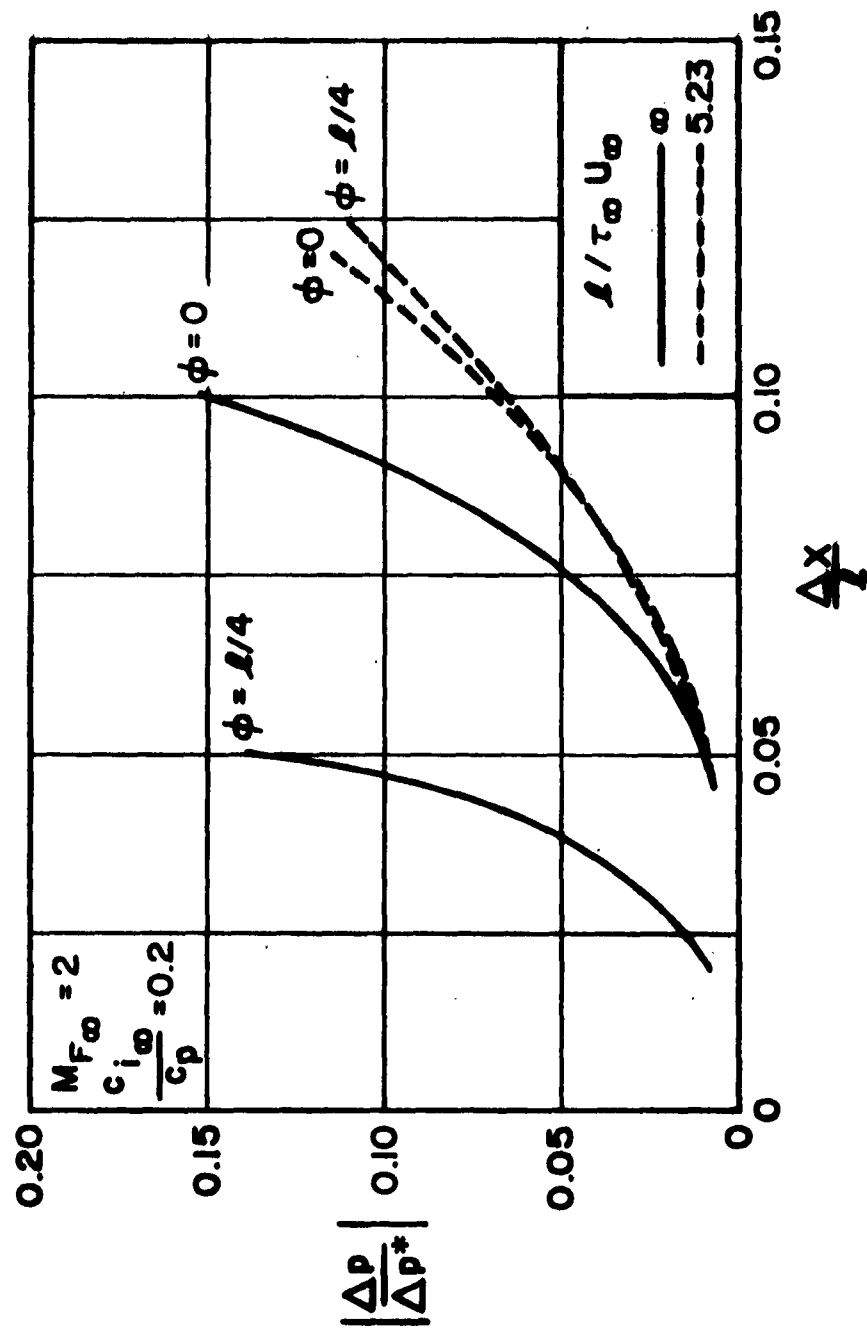


Figure 4. Error in Pressure, (a) $\rightarrow \infty$

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