DISCONTINUOUS SOLUTIONS FOR NONEQUILIBRIUM SUPERSONIC FLOWS

by

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SUMMARY

Generalized solutions with weak or strong discontinuities (that is, discontinuities in the derivatives or the variables themselves, respectively) are considered for nonequilibrium supersonic flows. The curves with weak discontinuities are shown to be the characteristics of the system of equations. The interdependence of the discontinuities for several variables are discussed.
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NOTATION

\( p \) pressure
\( \rho \) density
\( \alpha \) degree of dissociation (mass concentration of atoms)
\( T \) temperature
\( h \) specific enthalpy
\( S \) specific entropy
\( \vec{q} \) flow velocity vector
\( R \) gas constant per unit mass referred to diatomic gas
\( Q \) external heat added to or removed from the flow
\( w \) mass production rate
\( x,y \) Cartesian coordinates
\( \psi(x,y) \) stream function
\( L \) characteristic distance for dissociation
\( \zeta \) vorticity
\( \varphi(x,y) \) equation of the curve C in Cartesian coordinates
\( \vec{C}_n \) normal vector of curve C
\( \vec{S}_n \) unit vector along streamline
\( \vec{n} \) unit vector normal to streamline
\( \epsilon \) angle between \( \vec{C}_n \) and \( \vec{n} \)
\( u,v \) velocity components in x and y directions
\( v \) equal to 1 for plane flow and 2 for axially symmetric flow
\( a_e \) equilibrium speed of sound
\( \gamma_f \) specific heat ratio for frozen flow
\( \gamma_{fr} \) specific heat ratio for partially frozen flow
\( a_{fr} \) \( \gamma_f \) \( p/\rho \), frozen speed of sound
\( \epsilon_{fr} \) partially frozen speed of sound, \( (\gamma_{fr} \ p/\rho) \)
\( \eta \) defined as any smooth test function which vanishes identically outside a subdomain R of G (Eq. 49)
\( \beta_{fr}^2 \) \( M_f^2 - 1 \)
1. **INTRODUCTION**

The application of the method of characteristics for the computation of a supersonic flow field in a reacting gas under nonequilibrium conditions has been considered by several authors (Refs. 1 - 5).

In any discussion of the integration of systems of first order quasi-linear partial differential equations of the hyperbolic type, two important points arise:

1) Which of the dependant variables can be prescribed arbitrarily along a given initial data line without over-determining the solutions?

2) Apart from the solution for which the dependent variables and their derivatives of various orders are continuous in the whole flow field, does this system admit any other solutions:

   a) for which the first derivatives of the dependent variables are discontinuous in some part of the flow field while the variables themselves are continuous (these solutions are called generalized solutions with weak discontinuities),

   b) for which some or all of the dependent variables themselves are discontinuous (these solutions are called generalized solutions with strong discontinuities).

3) If such generalized solutions are available, where do these discontinuities occur? Does the discontinuity for one of the dependent variables across a curve mean discontinuities in all other dependent variables across the same curve? Are the discontinuities in the various dependent variables across any curve independent of each other or are they interrelated?

It is often thought that question 2a) can be answered directly from the characteristic equation along a given characteristic curve (e.g. Ref. 3). This could lead to erroneous conclusions as will be shown in this paper since the only thing that the characteristic equation tells us is that the derivatives normal to the characteristic curve along which that particular equation is valid cannot be calculated from a knowledge of the variables on it; however, it cannot be automatically concluded that these derivatives could be arbitrarily prescribed, that is they can be discontinuous. As will be seen later in this paper, this element of arbitrariness about the normal derivatives is eliminated by the basic set of differential equations themselves even without the introduction of initial and boundary conditions. (See the Appendix and Section 5 for further details.)

Thus, in this paper, it is proposed to answer questions (2) and (3) for supersonic flow of reacting gases in nonequilibrium by a systematic analysis starting from the basic set of differential equations defining the flow field. As question (1) was dealt with in considerable detail in Ref. 3, it will not be considered in this note.
2. BASIC EQUATIONS

Even though consideration of a number of reacting species or nonequilibrium in internal modes such as vibration does not introduce any special difficulties, for simplicity, the discussion will be restricted to the dissociative nonequilibrium of a pure dissociating diatomic gas. The vibrational degrees are considered to equilibrate instantaneously with the translational and rotational degrees of freedom (Ref. 5). The basic steady flow equations for the thermodynamic and flow variables $p$, $\rho$, $\alpha$, $T$, $h$, $S$, $\bar{q}$, which are the pressure, density, atomic mass fraction, temperature, specific enthalpy, specific entropy and velocity can be written in vector notation as:

- Mass: \[
\frac{\partial p}{\partial t} + \rho \text{div} \bar{q} = 0 \quad (1)
\]

- Momentum: \[
\text{grad} \frac{q^2}{2} - \bar{q} \times \text{curl} \bar{q} + \frac{1}{\rho} \text{grad} p = 0 \quad (2)
\]

- Energy: \[
\frac{\partial h}{\partial t} - \frac{1}{\rho} \frac{\partial p}{\partial t} = 0 \quad (3)
\]

- Entropy: \[
T \text{grad} S = -\bar{q} \times \text{curl} \bar{q} + Q \text{grad} \alpha \quad (4)
\]

- Rate Equation: \[
\frac{\partial \alpha}{\partial t} = \psi(p, \rho, \alpha) L(p, \rho, \alpha) \quad (5)
\]

- Equation of State: \[
p = \rho RT (1 + \alpha) \quad (6)
\]

- Enthalpy: \[
h = h(p, \rho, \alpha) \text{ or } h(\alpha, T) \quad (7)
\]

The expressions for specific enthalpy $h$ and specific entropy $S$ for the kind of model gas considered are given in Ref. 5. In the above equations $\text{D} / \text{D}t = \text{grad}$ and explicit expressions for $Q$, $\psi$, $L$ in terms of $p$, $\rho$, $\alpha$ can be written.

The basic derivation of the rate equation was considered in considerable detail in Ref. 5. The momentum equation, Eq. (2) is written explicitly in terms of the vorticity vector $\text{curl} \bar{q}$ to facilitate the discussion.

We will further restrict our discussion to two dimensional or axially symmetric flows. The latter differs from the former only in the addition of a term in the continuity equation while all others are unaffected. The continuity equation will be of the form

- In Cartesian coordinates $x$, $y$: \[
\frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) + (v-1) \frac{\rho v}{y} = 0 \quad (1')
\]

- In streamline coordinates, $s$, $n$ ($s$ along streamlines and $n$ perpendicular to it): \[
\frac{\partial}{\partial s} (\rho q) + \rho q \frac{\partial}{\partial n} + \frac{v-1}{r} \rho q \sin \theta = 0 \quad (1'')
\]

In Eqs. (1'), (1'') $u$, $v$ are the $x$, $y$ components of the velocity, $q$ the speed, $\theta$ the streamline angle, $\delta = 1$ for plane flow and $\nu = 2$ for axially symmetric flows and $r$ is the radial distance from the center line of axial symmetry.
3. ANALYSIS

Leaving aside the solutions of this set of equations for which the dependent variables and their derivatives of various orders are continuous everywhere in a supersonic flow field, some interesting results about generalized solutions, that is, solutions with weak or strong discontinuities in certain parts of the flow field can be derived (Refs. 6, 7).

3.1 Weak Discontinuities

As the system of equations Eqs. (1) to (6) is of first order, generalized solutions with weak discontinuities imply discontinuities in the first derivatives of the dependent variables (Ref. 7).

Let \( C \) be a curve in the flow field with unit normal \( \mathbf{C}_n \).

Consider two points \( P_1 \) and \( P_2 \) in the immediate neighbourhood but on opposite sides of this curve and along the normal. The relation between the normal derivatives of the pressure \( p \) and velocity \( q \) across the curve \( C \) can be obtained by taking the dot product of the momentum, Eq. (2), with \( \mathbf{C}_n \).

\[
\mathbf{C}_n \cdot \text{grad} \left( \frac{q^2}{2} - \mathbf{C}_n \cdot \vec{q} \times \text{curl} \, \vec{q} + \frac{1}{\rho} \mathbf{C}_n \cdot \text{grad} \, p \right) = 0
\]

or

\[
\frac{d}{dC_n} \left( \frac{q^2}{2} \right) + \frac{1}{\rho} \frac{dp}{dC_n} - \mathbf{C}_n \cdot \vec{q} \times \text{curl} \, \vec{q} = 0 \tag{8}
\]

where the differentiation \( d/dC_n \) is along the normal to the curve \( C \).

Applying Eq. (8) at the points \( P_1 \) and \( P_2 \), taking their difference and letting \( P_1 \rightarrow P_2 \) on the curve \( C \), one obtains:

\[
q \left[ q_{C_n} \right] + \frac{1}{\rho} \left[ P_{C_n} \right] - \left[ \mathbf{C}_n \cdot \vec{q} \times \text{curl} \, \vec{q} \right] = 0 \tag{9}
\]

where

\[
\left[ q_{C_n} \right] = \lim_{P_1, P_2 \rightarrow P} \left[ \left( \frac{\partial q}{\partial C_n} \right)_{P_1} - \left( \frac{\partial q}{\partial C_n} \right)_{P_2} \right] \tag{10}
\]
and similarly for the other two terms. The direction of the vector $\vec{q} \times \text{curl} \vec{q}$ in plane or axially symmetric flows is normal to the streamlines and in the plane of flow or the meridian plane.

If $\vec{s}$, $\vec{n}$ denote unit vectors along and normal to streamlines, for $\vec{c}_n = \vec{s}$, the third term in Eq. (9) is zero, while for any other $\vec{c}_n \neq \vec{s}$, it is different from zero. In terms of the streamline coordinates $s, n$ and the variables $q, \theta$ speed and streamline angle,

$$\vec{q} \times \text{curl} \vec{q} = q \left( \frac{\partial q}{\partial n} - q \frac{\partial \theta}{\partial s} \right) \vec{n}$$

$$= q \zeta \vec{n}$$

where $\zeta$ is the vorticity. Thus

$$[\vec{c}_n \cdot (\vec{q} \times \text{curl} \vec{q})] = [\vec{c}_n \cdot q \zeta \vec{n}]$$

$$= q [\zeta \vec{c}_n \cdot \vec{n}] = q \cos \epsilon [\zeta]$$

since the dependent variable $q$ and the angle between $\vec{c}_n$ and $\vec{n}$, $\epsilon$ are continuous across the curve $C$, while $\zeta$ which contains derivatives of $q$ and $\theta$ need not be continuous. Thus Eq. (9) is finally written as:

$$q [a_{C_n}] + \frac{1}{\rho} [p_{C_n}] - q \cos \epsilon [\zeta] = 0$$

### 3.1.1 Some General Results

Some results on the inadmissibility of discontinuous derivatives of certain variables across certain curves valid for reacting, non-reacting, rotational and irrotational flows will be first derived. It will be seen that these are a direct consequence of the basic set of partial differential equations defining the flow field and no initial or boundary conditions are introduced in their derivation.

(a) $[\zeta] = 0$ everywhere except across streamlines:

Let the equation of the curve $C$ in Cartesian coordinates be $\varphi(x, y) = 0$. $\varphi$ must have continuous partial derivatives of first order and $\varphi_x^2 + \varphi_y^2 \neq 0$. Then the derivatives of any quantity along and normal to $C$ are given by the operators:

\begin{align*}
\text{along } C: \quad & \varphi_y \frac{\partial}{\partial x} - \varphi_x \frac{\partial}{\partial y} \\
\text{across } C: \quad & \frac{d}{dC_n} = \varphi_x \frac{\partial}{\partial x} + \varphi_y \frac{\partial}{\partial y}
\end{align*}

(14)

Since the variables are continuous along the curve $C$ and also their derivatives in the direction of $C$, the jumps in the derivatives of the $x, y$ components of the velocity $u, v$ and pressure $p$ are related through
From the $x,y$ components of the momentum equation,

$$
\begin{align*}
\varphi_y [u_x] - \varphi_x [u_y] &= 0 \quad (15) \\
\varphi_y [v_x] - \varphi_x [v_y] &= 0 \quad (16) \\
\varphi_y [p_x] - \varphi_x [p_y] &= 0 \quad (17)
\end{align*}
$$

Multiplying Eq. (18) by $\varphi_x$ and Eq. (19) by $\varphi_x$ and subtracting, it can be shown with the aid of Eqs. (15) to (17), that

$$
(u \varphi_x + v \varphi_y) [u_y - v_x] = (\mathbf{q} \cdot \text{grad } \varphi)[\xi] = 0
$$
or

$$
q (\hat{s} \cdot \hat{c}_n) [\xi] = 0 \quad (20)
$$

where $\hat{s}$ is the unit vector along the streamlines. Thus the jump in the vorticity $[\xi]$ is zero except when the curve is the streamline itself in which case $\hat{s} \cdot \hat{c}_n = 0$ and thus $[\xi]$ need not be zero.

(b) $[\theta_n] = 0$, $[p_n] = 0$ across streamlines:

Applying the continuity equation Eq. (1") in streamline coordinates on either side of a streamline and taking the limit, one has

$$
q [\rho_s] + \rho [q_s] + \rho q [\theta_n] = 0 \quad (21)
$$

As the last term in Eq. (1") contains only variables, but no derivatives, it drops out. Since $\rho$, $q$ and so also their derivatives are continuous along streamlines $[\rho_s], [q_s]$ are zero leading to

$$
[\theta_n] = 0 \quad (22)
$$

Applying the $n$ component of the momentum equation in streamline coordinates $s, n$ on either side of a streamline and taking the limit

$$
\rho q^2 [\theta_s] + [p_n] = 0 \quad (23)
$$

Since the streamline angle $\theta$ and its derivative along the streamlines are continuous $[\theta_s] = 0$. Thus

$$
[p_n] = 0 \quad (24)
$$

Equations (22) and (24) show that no discontinuities in $p_n$ and $\theta_n$ are admissible across streamlines.
3.1.2 Reacting Gas Flows

(a) \([\alpha C_n] \neq 0\) only across streamlines:

Since the dissociated mass fraction \(\alpha\) as well as its derivative along a curve \(C\) are continuous, applying the operation in Eq. (14)

\[
\Phi_y [\alpha_x] - \Phi_x [\alpha_y] = 0
\] (25)

Applying the rate equation, Eq. (5) on either side of curve \(C\) and taking limits

\[
u [\alpha_x] + v [\alpha_y] = 0
\] (26)

Since \(\psi\) and \(L\) contain only the variables themselves but no derivatives. Equations (25), (26) show that

\[
[\alpha_y] \left(\frac{\omega y + \omega y}{r} \right) [\alpha_y] = \left(\frac{\omega x}{r} \right) [\alpha_x] \bigg|_{\alpha} \nabla \cdot \vec{S} \cdot \vec{C}_n/\psi_y = 0
\] (27)

from which, along with Eq. (25), one obtains

\[
[\alpha_y] = 0 = [\alpha_x] \text{ for } \vec{S} \cdot \vec{C}_n \neq 0
\]

Thus

\[
[\alpha C_n] = \Phi_x [\alpha_x] + \Phi_y [\alpha_y] = 0 \text{ for } \vec{S} \cdot \vec{C}_n \neq 0
\] (28)

It may be noted that since the rate equations for several reacting species and nonequilibrium in internal modes are all essentially of the type of Eq. (5) with the RHS being functions of the variables only, all of these can admit discontinuous normal derivatives across streamlines only.

(b) Other results:

For reacting gases, \(p\) can be written as a function of \(\rho, S, \alpha\) by eliminating the temperature \(T\) between \(p\) and \(S\), thus:

\[
p = p(\rho, S, \alpha)
\] (29)

From this equation, one has

\[
p C_n = (p_\rho)_S,\alpha C_n + (p_S)_\rho,\alpha S C_n + (p_\alpha)_\rho, S \alpha C_n
\] (30)

By taking the dot product of the entropy equation Eq. (4) by \(\vec{C}_n\), one has

\[
T S C_n = - q \cos \epsilon \zeta + Q \alpha C_n
\] (31)

where Eq. (11) is made use of. Eliminating \(S C_n\) from Eqs. (30), (31), one has

\[
[p C_n] = a_\tau \left[\rho C_n\right] - (p_S)_\rho,\alpha \qquad \cos \epsilon \zeta / T + \left\{ (p_\alpha)_\rho, S + (p_\alpha)_\rho, \alpha Q/T \right\} [\alpha C_n]
\] (32)
which relates the jumps in the normal derivatives across any curve \( C \). In the
above equation \( a^2_F = (p_S)_S \) is the partially frozen speed of sound for a
partially excited dissociating gas (Ref. 5).

Another relation between the jumps in the normal derivatives of
\( p, \rho, T \) and \( \alpha \) can be derived from the equation of state Eq. (6), namely

\[
[p_{C_n}] / \rho = [\rho_{C_n}] / \rho + [T_{C_n}] / T + [\alpha_{C_n}] / (1 + \alpha)
\]  

(33)

For undissociated and frozen flows, the jump relations are obtained by putting
\( \alpha \) zero and constant respectively in Eqs. (32), (33). For equilibrium flows,
\( \alpha \) is a function of \( p \) and \( \rho \) i.e. \( \alpha_e = \alpha(p, \rho) \) and thus the jump relations are
obtained by replacing derivatives of \( \alpha \) in terms of \( p \) and \( \rho \). This will modify
Eq. (32) such that \( a^2_F \) is replaced by \( a^2_e \), the equilibrium speed of sound.

3.1.3 Summary of Results

The results derived in Sections 3.1.1 and 3.1.2(a) suggest the
classification of the curves admitting discontinuous normal derivatives into
streamlines and others. For these two sets of curves, Eqs. (13, (31), (32) and
(33) will be simplified and it will be shown later that the other curves are
none else than the frozen Mach lines.

(a) Curve \( C \) is a streamline ( \( \vec{s} \cdot \vec{C}_n = 0, \epsilon = 0 \)):

It is already shown that for streamlines

\[
[q_n] = 0
\]  

(22)

\[
[p_n] = 0
\]  

(24)

Replacing the differentiation with respect to \( C_n \) by \( n \), one has

From Eq. (31)

\[
T [S_n] = - q \cos \epsilon \cdot [\xi] + q [\alpha_n]
\]  

(31')

Equation (13) reduces to

\[
[q_n] = \frac{1}{\rho} [\xi]
\]  

(34)

Equation (32) reduces to

\[
- a^2_F [\rho_n] = - (p_S)_S \alpha \cdot q [\xi] / T + \left\{ \left( (p_\alpha)_S + (p_\alpha)_S \right) \alpha \cdot q / T \right\} [\alpha_n]
\]  

(35)

Equation (33) reduces to

\[
[p_n] / \rho + [T_n] / T + [\alpha_n] / (1 + \alpha) = 0
\]  

(36)
One may note that for undissociated or frozen flows, the $\alpha$ term in Eqs. (31'), (35) and (36) disappears and the above equations reduce to

$$T \left[ S_\| \right] = - q \cos \epsilon [\xi]$$  \hspace{1cm} (31'')

$$a_f^2 \left[ \rho_n \right] = (p_b) \rho_n \alpha q [\xi]/T$$  \hspace{1cm} (35')

$$[\rho_n]/\rho + [T_n]/T = 0$$  \hspace{1cm} (36')

From Eqs. (31''), (34), (35') and (36'), it is seen that any jump in one variable determines all others uniquely, whereas for reacting flows Eqs. (31'), (34), (35), (36) show that no one jump uniquely determines all others, but any two will determine all others uniquely. They may be taken as $[q_n]$ and $[\alpha_n]$. Also note that streamlines are a set of characteristics for reacting gas flows, and also that no initial or boundary conditions are utilized in deriving the above results.

One very interesting result for undissociated gas flows is that if one has an initial condition that $\xi = 0$, $\xi$ remains zero everywhere and thus Eqs. (31''), (34), (35'), (36') show that none of the other variables admit any discontinuous normal derivatives across streamlines. Thus if one uses the definition of characteristic curves as those along which discontinuities can propagate, then the streamlines drop out as characteristic curves for undissociated flows with $\xi = 0$ initially i.e. irrotational flows. However from a mathematical point of view, streamlines are still characteristic curves for the set of Eqs. (1) to (5).

(b) Curve C is other than a streamline ($\vec{s} \cdot \vec{C}_n \neq 0$):

In this case, as shown earlier,

$$[\xi] = 0$$  \hspace{1cm} (37)

$$[\alpha_n] = 0$$  \hspace{1cm} (28)

Equation (31) reduces to

$$[S_{C_n}] = 0$$  \hspace{1cm} (31'' )

Equation (13) reduces to

$$\rho q [q_n] + [p_C] = 0$$  \hspace{1cm} (38)

Equation (32) reduces to

$$[p_{C_n}] = a_f^2 \left[ \rho_{C_n} \right]$$  \hspace{1cm} (39)

Equation (33) reduces to

$$(\gamma_f - 1) [p_{C_n}]/p = \gamma_f [T_{C_n}]/T$$  \hspace{1cm} (40)

where Eq. (39) is made use of and $\gamma_f$ is defined by the relation

$$a_f^2 = \gamma_f \frac{p}{\rho}$$  \hspace{1cm} (41)
to bring out the contrast with the undissociated gas flows. One may note that none of these results make use of any initial or boundary conditions and also that these equations themselves cannot determine whether $\theta_n$ is different from zero or not across curves other than streamlines. Also Eqs. (37) to (40) are equally valid for undissociated or frozen flows. While in the former case the frozen speed of sound and $\gamma_f$ are to be replaced in Eqs. (39) and (40) by the unambiguous speed of sound and the isentropic exponent, for frozen flows the appropriately frozen values of $\gamma_f$ and $a_f$ are to be used. Also for all flows, reacting or nonreacting, the above equations indicate that any one jump uniquely determines all others except $\theta_n$ as already noted. In other words, for both reacting and nonreacting flows, two jumps of which one should invariably be $\theta_n$ are required to uniquely determine all other jumps, in contrast with the situation for streamlines where any two could be chosen.

One interesting result when one makes use of the boundary condition $\theta_n = 0$ (for example flow around a smooth convex bend), is that these curves can still propagate discontinuities even for non-reacting flows. This seems to be the reason for indicating Mach lines (it will be shown below that these other curves are none else than Mach lines) as the only characteristic directions for irrotational flows in all Gasdynamics textbooks dealing with the application of the method of characteristics to gasdynamics problems.

To show that these curves are none other than Mach lines, one proceeds as follows:

Equations (38), (39) with the aid of the definition of $d/d\zeta$ given in Eq. (14) lead to

$$\phi_x u [u_x] + \phi_y u [u_y] + \phi_x v [v_x] + \phi_y v [v_y] + a_f^2 \left( \phi_x [\rho_x] + \phi_y [\rho_y] \right) / \rho = 0 \quad (42)$$

Also applying the continuity equation Eq. (1') in cartesian coordinates on both sides of the curve C and taking the limit

$$u [\rho_x] + v [\rho_y] + \rho \left( [u_x] + [v_y] \right) = 0 \quad (43)$$

The last term in Eq. (1') drops out since it contains only variables but no derivatives. Multiplying Eq. (15) by $\phi_y$ and Eq. (16) by $\phi_x$ and adding

$$\phi_y^2 [u_x] - \phi_x^2 [v_y] = - [\xi] \phi_y \phi_x = 0 \quad (44)$$

since $[\xi] = 0$ for all curves C other than streamlines. Since $\rho$ is continuous along $C$, so also its derivative along $C$ and thus

$$\phi_y [\rho_x] - \phi_x [\rho_y] = 0 \quad (45)$$

With the aid of Eqs. (43) to (45), Eq. (42) can be reduced to

$$(u^2 - a_f^2) \phi_x^2 + 2 u v \phi_x \phi_y + (v^2 - a_f^2) \phi_y^2 = 0 \quad (46)$$

which is the equation giving the frozen Mach lines as the other curves where discontinuous normal derivatives are admissible. As is already pointed out, for nonreacting flows, the frozen speed of sound is to be replaced by the ordinary speed of sound.
3.2 Strong Discontinuities

For a system of equations of nth order, generalized solutions with strong discontinuities are defined as solutions with discontinuities in the variables themselves or in their derivatives up to the (n-1)th order (Ref. 7). Let \( u \) be a function of \( x, y \) and have continuous derivatives of all orders everywhere in a domain \( G \) except on a curve \( u(x,y) = 0 \). Let the function \( u \) satisfy the linear partial differential equation

\[
L(u) = A \frac{\partial u}{\partial x} + B \frac{\partial u}{\partial y} + Cu = 0
\]

(47)

where \( A, B, \) and \( C \) are functions of \( x \) and \( y \) only.

Define an adjoint operation \( L^* \) such that (see Ref. 8 for a discussion of generalized adjoint operator)

\[
\eta L(u) - u L^*(\eta)
\]

(48)

is a divergence expression. \( u \) is said to be a generalized solution of the differential equation \( L(u) = 0 \), if

\[
\iint_R [\eta L(u) - u L^*(\eta)] \, dx \, dy = 0
\]

(49)

where \( \eta \) is any smooth test function which vanishes identically outside a subdomain \( R \) of \( G \). This definition can be extended to the case of quasi-linear equation with one dependent variable and also to systems of quasi-linear equations for several dependent variables provided they have the form of divergence equations or conservation laws, for example,

\[
L(u) = p_x(x,y,u) + q_y(x,y,u) + n(x,y,u) = 0
\]

(50)

where \( p, q, n \) are twice continuously differentiable function vectors of \( x, y \) in \( G \) and of \( u \) in some domain: Let the curve \( C \) divide the domain \( R \) into two subdomains \( R_1 \) and \( R_2 \) and then applying Eq. (49) in \( R_1 \) and \( R_2 \) and using Gauss's theorem the relation between the jump discontinuities \( p \) and \( q \) are connected with \( \phi_x, \phi_y \) as
\[ \int \int_{R} [\eta L(u) - uL*(\eta)] \, dx \, dy = \int \int_{R} (\eta_{x} + (q\eta)_{y}) \, dx \, dy \]
\[ = \int_{C} \eta (\varphi_{x}[p] + \varphi_{y}[q]) \, ds \]
\[ = 0 \quad \text{(51)} \]

where \([\eta]\) again denotes jump conditions. As this should be true for any \(\eta\)

\[ \varphi_{x}[p] + \varphi_{y}[q] = 0 \quad \text{(52)} \]

(Further details may be obtained from Ref. 7).

Equations (1) to (3) may be written in Cartesian coordinates as

\[ (\rho u)_{x} + (\rho v)_{y} = 0 \quad \text{(53)} \]
\[ \rho u_{x} + \rho v_{y} + p_{x} = 0 \quad \text{(54)} \]
\[ \rho u_{v} + \rho v_{v} + p_{y} = 0 \quad \text{(55)} \]
\[ u \, h_{x} + v \, h_{y} - \frac{u}{\rho} p_{x} - \frac{v}{\rho} p_{y} = 0 \quad \text{(56)} \]

Equations (54) and (55) with the aid of Eq. (53) can be rewritten as

\[ (p + \rho u^{2})_{x} + (\rho uv)_{y} = 0 \quad \text{(54') \text{ (55')}} \]

Eliminating \(p\) from Eq. (56) with the aid of Eqs. (54) and (55) and making use of Eq. (53),

\[ uh_{x} + vh_{y} + u^{2}u_{x} + uv u_{y} + uv v_{x} + v^{2}v_{y} = 0 \]
\[ \rho u_{x} + \rho v_{y} + \rho(u^{2}/2)_{x} + \rho v(u^{2}/2)_{y} + \rho(u^{2}/2)_{x} + \rho v(v^{2}/2)_{y} = 0 \]

or

\[ [\rho u \left( h + \frac{u^{2} + v^{2}}{2} \right)]_{x} + [\rho v \left( h + \frac{u^{2} + v^{2}}{2} \right)]_{y} = 0 \quad \text{(57)} \]

Comparing Eqs. (53), (54), (55), (57) with Eq. (50) and applying the criterion of strong solution, the following relations between the jumps can be obtained in a similar way to that used to obtain (52). For example

\[ 0 = \int \int_{R} \left\{ \eta [\rho (u)_{x} + (\rho v)_{y}] + [\rho u_{x} + \rho v_{y}] \right\} \, dx \, dy \]
\[ = \int \int_{R} \left\{ (\eta \rho u)_{x} + (\eta \rho v)_{y} \right\} \, dx \, dy = \int_{C} \eta \left\{ \varphi_{x} [\rho u] + \varphi_{y} [\rho v] \right\} \, ds \quad \text{(58)} \]
Hence

$$\varphi_x [p] + \varphi_y [r] = 0 \quad (59)$$

Similarly from Eqs. (54'), (55'), (57)

$$\varphi_x [p + pu^2] + \varphi_y [puv] = 0 \quad (60)$$

$$\varphi_x [puv] + \varphi_y [p + pv^2] = 0 \quad (61)$$

$$\varphi_x \left[ pu \left( h + \frac{u^2 + v^2}{2} \right) \right] + \varphi_y \left[ pv \left( h + \frac{u^2 + v^2}{2} \right) \right] = 0 \quad (62)$$

To understand the meaning of Eqs. (59) to (62), let the curve be $$\varPhi(x,y) = x$$ so that $$\varphi_y = 0$$, $$\varphi_x = \text{constant} \neq 0$$. Then Eqs. (59) - (62) simplify to

$$[pu] = 0 \quad (63)$$

$$[p + pu^2] = 0 \quad (64)$$

$$[puv] = 0 \quad (65)$$

$$[pu \left( h + q^2/2 \right)] = 0 \quad (66)$$

or

$$p_1 u_1 = p_2 u_2 \quad (67)$$

$$p_1 + p_1 u_1^2 = p_2 + p_2 u_2^2 \quad (68)$$

$$p_1 u_1 v_1 = p_2 u_2 v_2 \quad (69)$$

$$p_1 u_1 \left( h_1 + \frac{q_1^2}{2} \right) = p_2 u_2 \left( h_2 + \frac{q_2^2}{2} \right) \quad (70)$$
By virtue of Eq. (67), Eqs. (69) and (70) reduce to

\[ \nu_1 = \nu_2 \]  \hspace{1cm} (71)
\[ h_1 + \frac{q_1^2}{2} = h_2 + \frac{q_2^2}{2} \]  \hspace{1cm} (72)

Taking the dot product of \( \rho q \) and Eq. 4 for the entropy

\[ \rho u S_x + \rho v S_y = \frac{\rho Q}{T} u \alpha_x + \frac{\rho Q}{T} v \alpha_y \]  \hspace{1cm} (73)

which may be rewritten with the aid of Eq. (53) as

\[ \left[ \rho u \left( S - \frac{Q \alpha}{T} \right) \right]_x + \left[ \rho v \left( S - \frac{Q \alpha}{T} \right) \right]_y \]  \hspace{1cm} (73')

from which as before

\[ \varphi_x \left[ \rho u \left( S - \frac{\rho Q \alpha}{T} \right) \right] + \varphi_y \left[ \rho v \left( S - \frac{\rho Q \alpha}{T} \right) \right] = 0 \]  \hspace{1cm} (74)

For \( \varphi_y = 0 \),

\[ \left[ \rho u \left( S - \frac{\rho Q \alpha}{T} \right) \right] = 0 \]  \hspace{1cm} (75)

or

\[ \rho_1 u_1 S_1 - \rho_2 u_2 S_2 = \frac{\rho_1 u_1 Q_1 \alpha_1}{T_1} - \frac{\rho_2 u_2 Q_2 \alpha_2}{T_2} \]  \hspace{1cm} (76)

Using Eq. (67), Eq. (76) gives

\[ S_1 - S_2 = \frac{Q_1 \alpha_1}{T_1} - \frac{Q_2 \alpha_2}{T_2} \]  \hspace{1cm} (77)

From the equation of state, Eq. (6) and Eq. (68)

\[ p_1 - p_2 = \rho_1 R T_1 \frac{(1 + \alpha_1)}{u_1} - \rho_2 R T_2 \frac{(1 + \alpha_2)}{u_1} \]

or

\[ \frac{R T_1 (1 + \alpha_1)}{u_1} - \frac{R T_2 (1 + \alpha_2)}{u_2} = u_2 - u_1 \]  \hspace{1cm} (78)

Equations (67), (68), (71) and (72) are the well-known oblique shock-wave relations; while Eqs. (59) to (62) give the relations for any curved shock. This section may be closed by noting that in the case of strong discontinuities, the curves where they can occur are not characteristics. It is also not possible simply from these equations to determine the shape of such curves.
Examples will be given for the simpler case of weak discontinuities. As an illustration of the results of section 3.1, consider the flow around a smooth convex corner AB with constant flow properties upstream of the corner.

At points A and B while the streamline angle \( \theta \) is continuous, its derivative may or may not be continuous. The curvature is definitely discontinuous. Thus there can be discontinuities in the normal derivatives of the flow variables across the frozen Mach lines emanating from the points A and B across which Eqs. (68) to (40) apply. This is so since it was shown in Section 3.1.3(b) that whether \([\theta_C]\) is different from zero or not, Eqs. (38) to (40) would still give jumps if one of the other variables has a jump discontinuity in its normal derivative.

Equation (38) may be written in terms of the \( x, y \) components of the velocity \( u, v \) as

\[
u [\mathbf{C}_n] + v [\mathbf{C}_n] + \frac{1}{\rho} [\mathbf{P}_n] = 0
\]  

(79)

Further \( u, v, \theta \) derivatives are related as

\[
\frac{u [\mathbf{C}_n] - v [\mathbf{C}_n]}{u^2 + v^2} = [\theta_C]
\]

(80)

Since \( v = 0 \) at point A, Eqs. (79) and (80) give

\[
[\mathbf{V}_C] = u [\theta_C]
\]

(81)

\[
\rho u [\mathbf{C}_n] = [\mathbf{P}_n]
\]

(82)

In this case the geometry of the problem, that is, a knowledge of the variation of \( \theta \) is enough to calculate \([\mathbf{V}_C]\). But there does not seem to be any way by which \([\mathbf{P}_n]\) or \([\mathbf{C}_n]\) can be calculated purely from the equations. One may have to appeal to some physical reasoning.
Consider as a further example the flow around a sharp convex corner with the flow variables again constant upstream of the corner. In this case $\theta$ is discontinuous at the corner since $\theta$ changes abruptly from zero to $\theta$ at $O$. Also the derivative of $\theta$ at $O$ is not defined therefore Eq. (81) has no meaning. However, by inserting an expansion fan centered at $O$ whose head and tail are inclined to the flow at the Mach angles appropriate to the upstream and downstream uniform flows, one may say that the flow is smoothed out far from the corner. For the flow above some streamline $\psi$, one may apply the criterion as before. However, the corner itself is a forbidden zone.

Consider further the flow in a divergent nozzle $AB'A'B'$ where the upstream and downstream portions are parallel, that is, the flow is parallel upstream of $AOA'$, where $A$ and $A'$ are the frozen Mach lines emanating from $A$ and $A'$ on the walls and inclined to the flow at the upstream frozen Mach angle. Also downstream of $CO'C'$, $C'O'$ and $C'O'$ are Mach lines emanating from $O'$ and inclined at the downstream frozen Mach angle. At points $A$, $A'$, $C$, $C'$ one may have a discontinuity in the derivatives of the streamline angle $\theta$ and Eqs. (81) and (82) again hold.

Finally, consider the free-jet expansion of a reacting supersonic flow through a nozzle. For the nozzle exit pressure $P_e$ slightly greater than the plenum chamber pressure $P_p$, expansion fans will be set up at the corners at the exit plane. Some distance downstream of the corner at the free-jet boundary, which is a streamline, all the variables are
continuous. The vorticity $\zeta$ on either side of this boundary streamline will be different making $[\zeta] \neq 0$. Thus from Eqs. (31') and (34) to (36), the discontinuities in the derivatives of the other variables can be determined provided one other quantity like $[\alpha_n]$ or $[T_n]$ are known.

5. DISCUSSION

It was pointed out in the introduction that one can arrive at erroneous results by inferring from the characteristic equations as to which variables can have discontinuous normal derivatives across a given characteristic curve. As an example, consider the $s$ component of the momentum equation

$$\rho \frac{q}{s} q_s + p_s = 0$$

(83)

which is in characteristic form along streamlines. From this one may conclude that $p$ and $q$ can admit discontinuous normal derivatives across streamlines as done in Ref. 3. But the results of Section 3.1.1(a) show that $p$ cannot admit any such discontinuities across streamlines.

As a further example by choosing $S$, $q$, $p$, $\alpha$ as basic variables, one gets the following characteristic equation valid along frozen Mach lines (see the Appendix for details):

$$\beta_f (T dS - Q d\alpha + q dq) + q^2 d\theta - \frac{df}{M_f} (\frac{1}{A_1} - \beta_f^2 A_2 - \beta_f^2 A_3) = 0$$

(84)

where $A_1$, $A_2$, $A_3$ are known functions of the variables. From this equation one may conclude that $S$, $\alpha$, $q$, $\theta$ can have discontinuous normal derivatives across frozen Mach lines. The results of Sections 3.1.2(a) and 3.1.3(b) show that $\alpha$ and $S$ cannot admit any such discontinuities.
Thus the analysis given in this paper is the correct approach to find out as to which variables can have weak discontinuities. This analysis further gives the relation between the discontinuities in the several variables.

6. CONCLUSIONS

In conclusion, one finds that

1. Across frozen Mach lines, the atomic mass fraction $\alpha$, and entropy $S$ cannot admit discontinuous derivatives while all other flow variables can. Also the vorticity $\zeta$ cannot have any discontinuity. These discontinuities are interrelated and any two, of which one should invariably be $[\theta_n]$, determine all others uniquely.

2. For streamlines, the analysis shows that $p$ and $\theta$ cannot admit discontinuous derivatives across them while all others can and again only two of them are independent while all others are uniquely determined by these. These two quantities may be chosen as $[q_n]$ and $[\alpha_n]$.

3. For undissociated flows, the initial condition of zero vorticity, i.e. irrotational flows, eliminates the streamline completely as a possible curve for discontinuous derivatives. The boundary condition $[\thetae_n] = 0$, however, leaves the Mach lines as possible curves of discontinuities.
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APPENDIX A

It was pointed out in the introduction in the main text that one can arrive at erroneous results by trying to conclude directly from the characteristic equations along given characteristic directions as to which variables could admit discontinuous derivatives across these curves. This point was already discussed to a certain extent in the Section 5 of the main text. It is proposed to give some more details in this Appendix.

First of all let us note that Eqs. (1) to (7) given in the text are the general equations defining the flow of a pure dissociated diatomic gas in dissociational nonequilibrium. They can be specialized to undissociated gas flow by putting all terms containing the dissociated mass fraction \( \alpha \) equal to zero. This is apart from any initial or boundary conditions such as the vorticity \( \zeta = 0 \) initially or that all the streamlines emanate from the same reservoir such that the stagnation enthalpy \( h_0 \) is the same everywhere. The prescription of these initial or boundary conditions further specialises to a particular kind of problem.

For the general problem (i.e. without the introduction of initial or boundary conditions) either with or without dissociation, one may ask: what is the number of characteristic directions? Which are the characteristic directions? What are the characteristic equations along these directions? Can these characteristic equations be written such that they contain differentials of different combinations of the fundamental variables along a given characteristic direction (for example combination of pressure \( p \), streamline angle \( \theta \) or speed \( q \) and streamline angle \( \theta \))? In this last question, one is not interested in the utility of these alternate equations in the numerical computation of the flow by the method of characteristics even though this point will be discussed.

For the purposes of this discussion the following definition of characteristic equations is adopted, namely,

"Characteristic equations are those containing all differentiations in a single direction; this direction is called the characteristic direction".

Let us restrict our attention to two-dimensional or axially symmetric steady flows. Equations (1) to (6) written in the streamline coordinates are:

\[
\begin{align*}
\text{Mass continuity:} & \quad \frac{\partial}{\partial s} (pq) + pq \frac{\partial \theta}{\partial n} + \frac{v-1}{r} pq \sin \theta = 0 \quad (A1) \\
\text{s momentum:} & \quad pq \frac{\partial q}{\partial s} + \frac{\partial p}{\partial s} = 0 \quad (A2) \\
\text{n momentum:} & \quad pq \frac{\partial q}{\partial n} - pq \zeta + \frac{\partial p}{\partial n} = 0 \quad (A3) \\
\zeta = & \frac{\partial q}{\partial n} - q \frac{\partial \theta}{\partial s} \quad (A4) \\
\text{Equation (A3) may also be written without introducing } \zeta \text{ the vorticity as} & \quad \rho q^2 \frac{\partial \theta}{\partial s} + \frac{\partial p}{\partial n} = 0 \quad (A3')
\end{align*}
\]
Energy: \( \rho q \frac{\partial h}{\partial s} - q \frac{\partial p}{\partial s} = 0 \) (A5)

s-Entropy: \( T \frac{\partial s}{\partial s} = q \frac{\partial \alpha}{\partial s} \) (A6)

n-Entropy: \( T \frac{\partial s}{\partial n} = -q \xi + q \frac{\partial \alpha}{\partial n} \) (A7)

or \( = -q \left( \frac{\partial q}{\partial n} - q \frac{\partial \theta}{\partial s} \right) + q \frac{\partial \alpha}{\partial n} \) (A7')

Dissociation rate: \( q \frac{\partial \alpha}{\partial s} = \psi L \) (A8)

or \( \frac{\partial \alpha}{\partial s} = \frac{\psi L}{q} = w \) (A8')

One has further the following algebraic equations:

Equation of state: \( p = \rho RT (1 + \alpha) \) (A9)

Enthalpy: \( h = h(p, \rho, \alpha) \) or \( h(\alpha, T) \) (A10)

Entropy: \( S = S(\rho, T, \alpha) \) (A11)

All the variables occurring in the above equations are already defined in the main text. Explicit expressions for \( q, \psi, L, h, S \) are given in Ref. 5 for a pure dissociated diatomic gas. In the above, Eqs. (A1) to (A9) can be treated as eight equations for the eight unknowns \( p, \rho, T, \alpha, h, S, q, \theta \). If one wishes to make use of the definition of enthalpy \( h \) given in Eq. (A10) and of Entropy \( S \) given in Eq. (A11) one can show that Eqs. (A5) and (A6) are essentially the same and thus one of them may be dropped and also remove 'h' from the set of unknowns. Also one may note that the entropy \( S \) appears only in Eqs. (A6) and (A7) and thus \( S \) or \( \partial S/\partial s \) or \( \partial S/\partial n \) can be computed from Eqs. (A11), (A6), (A7) after solving the remaining set of equations for the remaining six variables \( p, \rho, T, \alpha, q, \theta \). However, we shall eliminate only the enthalpy \( h \) from Eq. (A5) through the use of Eq. (A10) and further eliminate \( \partial p/\partial s, \partial p/\partial s \) in the resulting equation with the aid of Eqs. (A1) and (A2). These manipulations lead to

\(-\rho q \left[ \rho h_{p, \alpha}^{-1} \right] \frac{\partial q}{\partial s} + \rho (h_{p})_{p, \alpha} \frac{\partial p}{\partial s} + \rho (h_{\alpha})_{p, \rho} \frac{\partial \alpha}{\partial s} = 0\)

or \(-q \left[ \rho h_{p, \alpha}^{-1} \right] \frac{\partial q}{\partial s} + \rho (h_{p})_{p, \alpha} \left[ \frac{1}{q} \frac{\partial q}{\partial s} - \frac{\partial \theta}{\partial n} - \frac{v-1}{r} \sin \theta \right] + (h_{\alpha})_{p, \rho} \frac{\partial \alpha}{\partial s} = 0\) (A12)

or by the definition of the partially frozen speed of sound \( a_{f}^{-2} = -\left( \frac{h_{p} - 1/\rho}{h_{p}} \right) \)

one has

\( \left( \frac{q^{2}}{a_{f}^{2} - 1} \right) \frac{\partial q}{\partial s} - q \frac{\partial \theta}{\partial n} + \frac{q h_{w}}{ph_{p}} - \frac{v-1}{r} q \sin \theta = 0 \) (A13)

where Eq. (A8') is made use of.
Also one may note that Eq. (A5) can be integrated with the aid of Eq. (A2) to yield the energy integral

\[ h + \frac{q^2}{2} = h_0(n) \]  

(A14)

where \( h_0(n) \) is to stress that it is a function of \( n \) only. However, this equation is no better than (A5) as long as one does not wish to use any initial conditions (e.g. that initially the flow emanates from a region where \( h_0 \) is the same on all streamlines and thus \( h_0 \) is a pure constant).

Thus for the general problem, one has seven equations (A2), (A3'), (A4), (A6), (A7'), (A8'), (A9) for the seven unknowns \( p, \rho, T, \alpha, S, q, \theta \). One of these equations is an algebraic equation; the remaining six are first order partial differential equations. According to the theory of partial differential equations of the hyperbolic type, this system can be written into six characteristic equations along six characteristic directions (Ref. 7). Some of these characteristic directions may have multiplicity.

It is readily seen from the definition of characteristic directions adopted above that Eqs. (A2), (A6), (A8') are already in characteristic form along the streamlines. Thus streamlines are characteristic curves for this system. Also it may be noted that it has a multiplicity of 3 so far. To determine the remaining characteristic directions and the characteristic equations along them, let us define the coordinate \( \xi \) along this direction so that a total differential of any quantity along this direction may be written in terms of the partial differentials along \( s, n \) as

\[ \frac{d}{d\xi} = \frac{ds}{d\xi} \frac{\partial}{\partial s} + \frac{dn}{d\xi} \frac{\partial}{\partial n} \]  

(A15)

Thus one has

\[ \frac{dp}{d\xi} = \frac{ds}{d\xi} \frac{\partial p}{\partial s} + \frac{dn}{d\xi} \frac{\partial p}{\partial n} \]  

(A16)

\[ \frac{dq}{d\xi} = \frac{ds}{d\xi} \frac{\partial q}{\partial s} + \frac{dn}{d\xi} \frac{\partial q}{\partial n} \]  

(A17)

\[ \frac{d\theta}{d\xi} = \frac{ds}{d\xi} \frac{\partial \theta}{\partial s} + \frac{dn}{d\xi} \frac{\partial \theta}{\partial n} \]  

(A18)

\[ \frac{dp}{d\xi} = \frac{ds}{d\xi} \frac{\partial p}{\partial s} + \frac{dn}{d\xi} \frac{\partial p}{\partial n} \]  

(A19)

\[ \frac{dS}{d\xi} = \frac{ds}{d\xi} \frac{\partial S}{\partial s} + \frac{dn}{d\xi} \frac{\partial S}{\partial n} \]  

(A20)

\[ \frac{d\alpha}{d\xi} = \frac{ds}{d\xi} \frac{\partial \alpha}{\partial s} + \frac{dn}{d\xi} \frac{\partial \alpha}{\partial n} \]  

(A21)

Equations (A3'), (A4), (A7') together with Eqs. (A16) - (21) give the characteristic directions and the characteristic equations valid along them as follows:-
Multiplying Eq. (A3') by $\frac{ds}{dl} \cdot \frac{dn}{dl}$ and using Eqs. (A18) and (A19), one has

$$\rho q^2 \left[ \frac{\partial}{\partial l} - \frac{dn}{dl} \frac{\partial}{\partial n} \right] \frac{dn}{dl} + \left[ \frac{dp}{dl} - \frac{ds}{dl} \frac{\partial p}{\partial s} \right] \frac{ds}{dl} = 0$$

or

$$\frac{dp}{dl} \cdot \frac{ds}{dl} + \rho q^2 \frac{dn}{dl} \cdot \frac{dn}{dl} - \left[ \rho q^2 \left( \frac{dn}{dl} \right)^2 \frac{\partial q}{\partial n} + \left( \frac{ds}{dl} \right)^2 \frac{\partial p}{\partial s} \right] = 0$$

or eliminating $\frac{\partial p}{\partial s}$ with the aid of Eq. (A2)

$$\frac{dp}{dl} \cdot \frac{ds}{dl} + \rho q^2 \frac{dn}{dl} \cdot \frac{dn}{dl} - \left[ \rho q^2 \left( \frac{dn}{dl} \right)^2 \frac{\partial q}{\partial n} - \rho q \left( \frac{ds}{dl} \right)^2 \frac{\partial q}{\partial s} \right] = 0 \quad (A22)$$

Further eliminating $\frac{\partial q}{\partial s}$ with the aid of Eq. (A13), one obtains,

$$\frac{dp}{dl} \cdot \frac{ds}{dl} + \rho q^2 \frac{dn}{dl} \cdot \frac{dn}{dl} - \rho q \left[ \left( \frac{dn}{dl} \right)^2 \frac{\partial q}{\partial n} - \left( \frac{ds}{dl} \right)^2 \frac{\partial q}{\partial s} \right] = 0$$

Simplifying Eq. (A23) gives

$$\frac{dp}{dl} \cdot \frac{ds}{dl} + \rho q^2 \frac{dn}{dl} \cdot \frac{dn}{dl} - \rho q \left[ \left( \frac{dn}{dl} \right)^2 \frac{\partial q}{\partial n} - \left( \frac{ds}{dl} \right)^2 \frac{\partial q}{\partial s} \right] = 0$$

From Eq. (A24), the condition for it to be of characteristic form is that the coefficient of the partial differential $\partial \theta / \partial n$ be zero, i.e.

$$\left( \frac{dn}{dl} \right)^2 - \frac{1}{\beta^2_f} \left( \frac{ds}{dl} \right)^2 = 0$$

i.e.

$$\frac{ds/dl}{dn/dl} = \pm \beta_f^2 \quad (A25)$$

where

$$\beta_f^2 = M_f^2 - 1 \quad (A26)$$

Similarly multiplying Eq. (A7') by $\frac{ds}{dl} \cdot \frac{dn}{dl}$ and making use of Eqs. (A17), (A18), (A20) and (A21), one has

$$T \frac{ds}{dl} \left[ \frac{ds}{dl} - \frac{ds}{ds} \frac{\partial S}{\partial s} \right] + q \frac{ds}{dl} \left[ \frac{dq}{dl} - \frac{ds}{dl} \frac{\partial q}{\partial s} \right] - q^2 \frac{dn}{dl} \left[ \frac{\partial \theta}{\partial l} - \frac{dn}{dl} \frac{\partial \theta}{\partial n} \right]$$

$$- q \frac{ds}{dl} \left[ \frac{\partial \alpha}{\partial l} - \frac{ds}{dl} \frac{\partial \alpha}{\partial s} \right] = 0$$
or
\[ \frac{ds}{dl} \left[ T \frac{ds}{dl} - Q \frac{d\alpha}{dl} + q \frac{dq}{dl} \right] - q^2 \frac{dn}{dl} \cdot \frac{d\theta}{dl} - \left( \frac{ds}{dl} \right)^2 \left[ T \frac{ds}{dl} - Q \frac{d\alpha}{dl} \right] \]
\[ - q \left( \frac{ds}{dl} \right)^2 \frac{dq}{ds} + q^2 \left( \frac{dn}{dl} \right)^2 \frac{d\theta}{dn} = 0 \] (A27)

The third term on the LHS in Eq. (A27) is zero due to Eq. (A6). Replacing \( \frac{dq}{ds} \) in Eq. (A27) with the aid of Eq. (A13), one has

\[ \frac{ds}{dl} \left[ T \frac{ds}{dl} - Q \frac{d\alpha}{dl} + q \frac{dq}{dl} \right] - q^2 \frac{dn}{dl} \cdot \frac{d\theta}{dl} + \left( \frac{dn}{dl} \right)^2 q^2 \frac{d\theta}{dn} \]
\[ - \frac{q}{\beta_f^2} \left( \frac{ds}{dl} \right)^2 \left\{ q \frac{d\theta}{dn} - \frac{q h \alpha^w}{\rho \phi_p} + \frac{v-1}{r} q \sin \theta \right\} = 0 \] (A28)

Rearranging the terms in Eq. (A28), one has

\[ \frac{ds}{dl} \left[ T \frac{ds}{dl} - Q \frac{d\alpha}{dl} + q \frac{dq}{dl} \right] - q^2 \frac{dn}{dl} \cdot \frac{d\theta}{dl} + q^2 \frac{d\theta}{dn} \left[ \left( \frac{dn}{dl} \right)^2 \frac{1}{\beta_f^2} \left( \frac{ds}{dl} \right)^2 \right] \]
\[ + \frac{q}{\beta_f^2} \left( \frac{ds}{dl} \right)^2 \left[ h \frac{\alpha^w}{\rho \phi_p} - \frac{v-1}{r} \sin \theta \right] = 0 \] (A29)

The condition for Eq. (A29) to be of the characteristic form is that the coefficient of \( \partial \theta/\partial n \) in it be zero i.e.

\[ \left( \frac{dn}{dl} \right)^2 \frac{1}{\beta_f^2} \left( \frac{ds}{dl} \right)^2 = 0 \]

i.e.

\[ \frac{ds}{dl} \frac{dn}{dl} = \pm \beta_f \]

For the direction \( l \) satisfying Eq. (A25), one can show that

\[ \frac{ds}{dl} = \pm \beta_f/M_f \] (A30)

and

\[ \frac{dn}{dl} = \pm \frac{1}{M_f} \] (A31)

Substituting Eqs. (A25), (A30) and (A31) in Eqs. (A24) and (A29) one obtains two sets of characteristic equations valid along the frozen Mach lines, namely

\[ \pm \frac{\beta_f}{M_f} \frac{dp}{dl} + \frac{1}{M_f} \rho q^2 \frac{d\theta}{dl} + \rho q^2 \frac{dM}{dl} \left[ \frac{h \alpha^w}{\rho \phi_p} - \frac{v-1}{r} \sin \theta \right] = 0 \] (A32)

In the literature, this is the equation normally given. Since these equations contain differentials only in two variables \( p \) and \( \theta \), they can be readily solved by numerical methods for \( p \) and \( \theta \) at a third point knowing these values at two other points.
Equation (A29) reduces with the aid of Eqs. (A25), (A30), (A31) to
\[ \pm \frac{\beta_f}{M_f} \left[ T \frac{dS}{dl} - Q \frac{d\alpha}{dl} + q \frac{dq}{dl} \right] - \frac{q^2}{M_f} \frac{d\theta}{dl} + \frac{q^2}{M_f^2} \left[ \frac{h\alpha}{\rho \rho - \frac{v-1}{r} \sin \theta} \right] = 0 \quad (A33) \]

This is the other set of equations valid along frozen Mach lines. But this contains differentials in four variables \( S, \alpha, q, \theta \) while there are only two equations. Thus if one wishes to use this combination of variables it will be difficult to solve the problem numerically. This is the equation given in the discussion in the main text where it was pointed out that one may conclude that \( S, \alpha, q, \theta \) can have discontinuous derivatives across Mach lines. This is erroneous since it was shown in the text that \( S \) and \( \alpha \) cannot admit any such discontinuities across frozen Mach lines.

Let us summarise all the characteristic equations:

Along streamlines:
\[ \rho q \frac{dq}{ds} + \frac{dp}{ds} = 0 \quad (A34) \]
\[ T \frac{d\alpha}{ds} - Q \frac{d\alpha}{ds} = 0 \quad (A35) \]
\[ \frac{d\alpha}{ds} = w \quad (A36) \]
\[ \rho \frac{dp}{ds} - \frac{dp}{ds} = 0 \quad (A37) \]

Along frozen Mach lines:
\[ \pm \beta_f \frac{dp}{dl} + \rho q^2 \frac{d\theta}{dl} + \rho q^2 \frac{h\alpha}{\rho \rho - \frac{v-1}{r} \sin \theta} = 0 \quad (A38) \]
\[ \pm \beta_f \left[ T \frac{dS}{dl} - Q \frac{d\alpha}{dl} + q \frac{dq}{dl} \right] - \frac{q^2}{M_f} \frac{d\theta}{dl} + \frac{q^2}{M_f^2} \left[ \frac{h\alpha}{\rho \rho - \frac{v-1}{r} \sin \theta} \right] = 0 \quad (A39) \]

If one chooses \( p, q, \alpha \) as the basic set of variables, Eqs. (A34) (A36) and (A38) are to be used whereas if one chooses \( S, q, \theta, \alpha \) as the basic variables, Eqs. (A35), (A36) and (A39) are to be used in the numerical computation of the flow field by the method of characteristics. Also one may note that one does not have a characteristic equation involving differentials of \( q \) and \( \theta \) alone along frozen Mach lines, but one has in addition the differentials of \( S \) and \( \alpha \) also. Some statements in Ref. 3 seem to imply that one can have a characteristic equation involving differentials of \( q \) and \( \theta \) alone along frozen Mach lines.

For non-reacting flows, the above equations reduce to (by putting \( \alpha \) terms equal to zero),
\[ \rho q \frac{dq}{ds} + \frac{dp}{ds} = 0 \quad (A34) \]
Along streamlines:
\[ \frac{dS}{ds} = 0 \quad (A40) \]

Along frozen Mach lines:
\[ \pm \beta_f \frac{dp}{dl} + \rho q^2 \frac{d\theta}{dl} - \frac{v-1}{r} \frac{\rho q^2}{M_f} \sin \theta = 0 \quad (A41) \]
\[ \pm \beta_f \left[ T \frac{dS}{dl} + q \frac{dq}{dl} \right] - q^2 \frac{d\theta}{dl} - \frac{v-1}{r} \frac{q^2}{M_f} \sin \theta = 0 \quad (A42) \]

Note that Eqs. (A34) and (A40) show that for even irrotational flows, the streamlines are still characteristics. Only that as pointed out in the text, the initial condition of zero vorticity removes streamlines from the directions which can admit discontinuous derivatives.
Generalized solutions with weak or strong discontinuities (that is, discontinuities in the derivatives or the variables themselves, respectively) are considered for nonequilibrium supersonic flows. The curves with weak discontinuities are shown to be the characteristics of the system of equations. The interdependence of the discontinuities for several variables are discussed.
1. Method of Characteristics
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