Sonic Line in Nonequilibrium Nozzle Flows†

by

Duvvuri Tirumalesa*
University of Toronto, Toronto, Ontario, Canada

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An equation valid in the region where the partially frozen Mach number is near unity is derived for the flow of a gas which is in dissociational nonequilibrium but where vibration and rotation are in equilibrium with translation (partially excited). From the solution of this equation for nozzle flows, it is shown that the constant velocity curves in the sonic region are parabolic, and thus a parabolic arc can be taken as the initial data curve for supersonic flow computations when using the method of characteristics. The curves of the limiting characteristic, the partially frozen sonic line and the line of horizontal velocity are all shown to be parabolic. The results are valid for slight departures from equilibrium. Author

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* Faculty of Applied Science and Engineering, University of Toronto, Senior Research Fellow, presently at the University of Southern California, Dept. of Aerospace Engg., Los Angeles, Calif., U. S. A. (On leave from National Aeronautical Laboratory, Bangalore, India).

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Introduction:

It is well known that in supersonic reacting gas flows in non-equilibrium, the flow field can be computed by the method of characteristics when the flow parameters on an initial data curve are given (Refs. 1-5). In these computations the frozen Mach number plays a role similar to that of the usual Mach number in non-reacting flows. The computation of supersonic flows in a de Laval nozzle is in general carried out by taking the initial data curve as a line perpendicular to the nozzle axis at a point where the frozen Mach number is slightly greater than unity (Refs. 6, 7). The flow parameters at this point are obtained by a quasi-one dimensional analysis up to this point and are assumed to be constant on this initial data curve. No justification is given for taking the initial data curve to be of this shape. Also in the inverse nozzle problem, it would be of interest to know which part of the nozzle could be modified without affecting the upstream flow. In this note it is proposed to answer these questions by studying the flow in the partially frozen sonic region (i.e., the region where the partially frozen Mach number is near unity).

Analysis:

The analysis is resticted to a steady two-dimensional flow of a pure diatomic gas such as 0_2 giving a binary mixture of atoms and molecules. It is assumed that only dissociation is out of equilibrium while the vibrational and rotational modes are in equilibrium with translation. The dissociational rate equation can be shown to be (Ref. 8)

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$$\frac{D\alpha}{Dt} = \psi(p, \rho, \alpha)\ L(p, \rho, \alpha) \tag{1}$$

where

$$\psi(p, \rho, \alpha) = k_r\, \rho^2 (1+\alpha)\, \alpha^2 / m_a{}^2 \tag{2}$$

$$L(p, \rho, \alpha) = \frac{m_a}{2\rho} K_c \frac{(1-\alpha)}{\alpha^2} - 1 \tag{3}$$

$$\frac{D}{Dt} = \vec{q}\ .\ \text{grad}$$

p, ρ, α, T, $\vec{q}$ are the pressure, density, dissociated mass fraction, temperature and velocity, respectively. It may be noted that $1/\psi$ has the dimensions of time, and L = 0 for dissociational equilibrium. K_c is the equilibrium constant and is the ratio of the dissociation and recombination rate constants k_d and k_r, which are functions of temperature only and, m_a is the mass of atoms per unit mole.

Let the flow be a perturbation from a reference state, which may or may not be in equilibrium and therefore

$$\begin{aligned} p &= p^* \ (1+p') \\ \rho &= \rho^* \ (1+\rho') \\ \alpha &= \alpha^* \ (1+\alpha') \end{aligned} \tag{4}$$

where the starred and primed quantities correspond to the reference state values and perturbations, respectively. Then the product ψL may be expanded in a Taylor series about this reference state as

$$\psi L = (\psi L)^* + (\psi L)_{p^*} p^* p' + (\psi L)_{\rho^*} \rho^* \rho' + (\psi L)_{\alpha^*} \alpha^* \alpha' \tag{5}$$

where subscripts denote differentiation.

Thus

$$\frac{D}{Dt}\left(\frac{D\alpha}{Dt}\right) = (\psi L)_{\alpha^*}\left\{\frac{(\psi L)_{p^*}}{(\psi L)_{\alpha^*}}\frac{Dp}{Dt} + \frac{(\psi L)_{\rho^*}}{(\psi L)_{\alpha^*}}\frac{D\rho}{Dt} + \frac{D\alpha}{Dt}\right\} \tag{6}$$

By defining a local equilibrium value α_e of α by

$$L(p, \rho, \alpha_e) = 0 \tag{7}$$

one obtains

$$\frac{(\psi L)_{p^*}}{(\psi L)_{\alpha^*}} = -\alpha_{e p^*} \quad , \quad \frac{(\psi L)_{\rho^*}}{(\psi L)_{\alpha^*}} = -\alpha_{e \rho^*} \tag{8}$$

Substituting these in Eq. (6) gives

$$\frac{D}{Dt}\left(\frac{D\alpha}{Dt}\right) = (\psi L)_{\alpha^*}\left\{-\alpha_{e p^*}\frac{Dp}{Dt} - \alpha_{e\rho^*}\frac{D\rho}{Dt} + \frac{D\alpha}{Dt}\right\} \tag{9}$$

From the energy equation

$$\frac{Dh}{Dt} - \frac{1}{\rho}\frac{Dp}{Dt} = 0 \tag{10}$$

where $h = h(p, \rho, \alpha)$ is the enthalpy, one obtains,

$$h_\alpha \frac{D\alpha}{Dt} = -\left(h_p - \frac{1}{\rho}\right)\frac{Dp}{Dt} - h_\rho \frac{D\rho}{Dt} \tag{11}$$

Substituting for $D\alpha/Dt$ from Eq. (11) on both sides of Eq. (9) and using the continuity and momentum equations

$$\frac{D\rho}{Dt} + \rho \, \mathrm{div}\, \vec{q} = 0 \tag{12}$$

$$\vec{q} \cdot \frac{D\vec{q}}{Dt} + \frac{1}{\rho}\frac{Dp}{Dt} = 0 \tag{13}$$

one obtains,

$$\frac{D}{Dt}\left\{\frac{\rho h_\rho}{h_\alpha}\left[\mathrm{div}\,\vec{q} - \frac{1}{a_f^2}\,\vec{q} \cdot \frac{D\vec{q}}{Dt}\right]\right\} + G\left[\mathrm{div}\,\vec{q} - \frac{1}{a_e^2}\,\vec{q} \cdot \frac{D\vec{q}}{Dt}\right] = 0 \tag{14}$$

where $$G = (\psi L)_{\alpha *}\left(h_\rho + h_\alpha \alpha_{e\rho *}\right) / h_{\alpha *} \qquad (15)$$

and the partially frozen and equilibrium speeds of sound a_f and a_e are defined in Ref. 5 and are given by

$$a_f^{-2} = -(h_p - 1/\rho)/h_\rho \qquad (16)$$

$$a_e^{-2} = -(h_p + h_\alpha \alpha_{ep} - \frac{1}{\rho}) / (h_\rho + h_\alpha \alpha_{e\rho}) \qquad (17)$$

For flows with constant total enthalpy, one obtains from Eqs. (10), (13),

$$h + q^2/2 = \text{constant} = h^* + q^{*2}/2 \qquad (18)$$

where h may be replaced in terms of a_f^2 and a_e^2 as

$$2h = A\, a_f^2 = B\, a_e^2 \qquad (19)$$

with A and B given by.

$$A = \frac{2}{\gamma_f - 1} = \frac{\left[5 + \alpha + 2(1-\alpha)\frac{d\varepsilon_v}{dT}\right]\left[1 + \frac{2(1-\alpha)\varepsilon_v + 2\alpha\,\theta_D}{(7+3\alpha)T}\right]}{(1+\alpha)\left[1 + \frac{2(1-\alpha)}{(7+3\alpha)}\frac{d\varepsilon_v}{dT}\right]} \qquad (20)$$

$$B = \frac{2}{\gamma_e - 1} = \frac{\left\{\frac{2-\alpha}{2}\left[5+\alpha+2(1-\alpha)\frac{d\varepsilon_v}{dT}\right] + \alpha(1-\alpha)\left(\frac{1}{2} + \frac{\theta_D - \varepsilon_v}{T}\right)^2\right\}\left[1 + \frac{2(1-\alpha)\varepsilon_v + 2\alpha\,\theta_D}{(7+3\alpha)T}\right]}{\left\{1 + \frac{1}{7+3\alpha}\left[2(1-\alpha)\frac{d\varepsilon_v}{dT} + \alpha(1-\alpha^2)\left(\frac{3}{2} + \frac{\theta_D - \varepsilon_v}{T}\right)^2\right\}} \qquad (21)$$

$$\varepsilon_v = \theta_v / \left(e^{\theta_v/T} - 1\right)$$

θ_v, θ_D are the characteristic temperatures for dissociation and vibration, γ_f and γ_e in the above expressions are the partially frozen and equilibrium isentropic exponents, similar to γ for non-reacting gas flows (Ref. 3). However, γ_f and γ_e are not constant. From Eqs. (18) and (19), one obtains the following relations between the flow speed and partially frozen and equilibrium sound speeds

$$a_f^2 = (A^* a_f^{*2} + q^{*2} - q^2)/A \qquad (22)$$

$$a_e^2 = (B_f^* \, a_f^{*2} + q^{*2} - q^2)/B \qquad (23)$$

where B_f^* is the value of B evaluated at $q^* = a_f^*$.

Transonic equation for reacting gas flows:

For flows which are slightly out of equilibrium, it may be shown (Ref. 8) that the flow can be considered to be nearly isentropic, and hence one may introduce a perturbation velocity potential φ such that

$$q_x = q_* + u' = a_f^* + \varphi_x \qquad (24)$$

$$q_y = v' = \varphi_y$$

where the reference state is now that corresponding to $q^* = a_f^*$. Furthermore, in the transonic region (where the partially frozen Mach number is near unity) one may derive a simplified equation from Eq. (14) by the following transformation, (See Ref. 8 for details):

$$\xi = \beta x$$

$$\eta = \beta \tau^{1/2} y \qquad (25)$$

$$\beta \varphi(x, y) = \tau a_f^* \bar{\varphi}(\xi, \eta)$$

where τ is a perturbation parameter that can be related to the quantity $\varepsilon / H_0 \beta$. Here $\varepsilon = H_0/R_0$, where H_0 is the height of the nozzle at the throat, and R_0 is the radius of curvature at the throat ; $1/\beta$ is the dissociational relaxation length and β is given by

$$\beta = (\psi L)_{\alpha *} \left(h_{\rho *} + h_{\alpha *} \alpha_{e \rho *} \right) / a_f^* h_{\rho *} \qquad (26)$$

In the limits of equilibrium and frozen flows, β tends to $-\infty$ and 0, respectively.

Also by writing

$$p = p^* (1 + \Upsilon p')$$

$$\rho = \rho^* (1 + \Upsilon \rho')$$

$$\alpha = \alpha^* (1 + \Upsilon \alpha') \qquad (27)$$

one can show that

$$A = A^* (1 + \Upsilon A')$$

$$B = B_f^* (1 + \Upsilon B')$$

$$\frac{\rho h_\rho}{h_\alpha} = \frac{\rho^* h_{\rho^*}}{h_{\alpha^*}} (1 + \Upsilon R_1') \qquad (28)$$

$$\rho (h_\rho + h_\alpha \alpha_{e\rho^*}) = \rho^* (h_{\rho^*} + h_{\alpha^*} \alpha_{e\rho^*}) (1 + \Upsilon R_2')$$

where A', B', R_1', R_2' are at most order unity (Ref. 8). Substituting from Eqs. (22) through (28) in Eq. (14) and simplifying, one obtains,

$$\Upsilon^2 \frac{\partial}{\partial \xi}\left\{-P\, \bar{\varphi}_\xi\, \bar{\varphi}_{\xi\xi} + \bar{\varphi}_{\eta\eta}\right\} - \left[M \Upsilon \bar{\varphi}_{\xi\xi} - N \Upsilon^2 \bar{\varphi}_\xi \bar{\varphi}_{\xi\xi} + \Upsilon^2 \bar{\varphi}_{\eta\eta}\right] + O(\Upsilon^3) = 0 \qquad (29)$$

where

$$P = 2(A^* + 1)/A^*$$

$$M = 1 - (a_f^* / a_e^*)^2 = 1 - B_f^*/A^* \qquad (30)$$

$$N = 2 (a_f^* / a_e^*)^2 (1 + a_f^{*2}/B_f^* a_e^{*2}). = P B_f^*/A^*$$

To order Υ, this gives

$$\bar{\varphi}_{\xi\xi} = 0$$

or

$$\bar{\varphi}_\xi = f(\eta) \qquad (31)$$

where $f(\eta)$ is a function of η alone showing that to this order $\bar{\varphi}_\xi$ is a function of η alone. But in general, the parameter M is of order Υ. Thus to order Υ^2, one has

$$\frac{\partial}{\partial \xi}\left\{-p\,\overline{\varphi}_{\xi}\,\overline{\varphi}_{\xi\xi}+\overline{\varphi}_{\eta\eta}\right\}_{,r}-\left\{\frac{M}{\Upsilon}\,\overline{\varphi}_{\xi\xi}-N\,\overline{\varphi}_{\xi}\,\overline{\varphi}_{\xi\xi}+\overline{\varphi}_{\eta\eta}\right\}=0 \quad (32)$$

or in the x, y coordinates,

$$\frac{\partial}{\partial x}\left\{-p\,\varphi_x\,\varphi_{xx}+\varphi_{yy}\right\}-\beta\left\{M\,\varphi_{xx}-N\,\varphi_x\,\varphi_{xx}+\varphi_{yy}\right\}=0 \quad (33)$$

This is the transonic equation for reacting gas flows valid in the region where the partially frozen Mach number is near unity.

<u>Solution for nozzle flows</u>:

Consider a nozzle symmetric with respect to the nozzle center-line taken as the x-axis. The perturbation velocity potential may be expanded as a polynomial in y in which the coefficients are functions of x. Because of the asymmetry of the y component of the velocity, only even powers of y will appear, thus

$$\varphi(x,y)=\varphi_0(x)+\frac{y^2}{2}\varphi_1(x)+\frac{y^4}{24}\varphi_2(x)+\ \ldots\ldots \quad (34)$$

In the sonic region, one can write

$$\varphi_{o_x}(x)=c\,x \quad (35)$$

where c is a positive constant, and the origin is taken as the sonic point. By substituting $\varphi(x,y)$ from Eq. (34) in Eq. (33) and using Eq. (35), one obtains

$$\varphi(x,y)=\frac{cx^2}{2}+\frac{y^2}{2}\left\{\frac{(N-p)c^2}{\beta}-Mc+Nc^2x+A_1e^{\beta x}\right\}$$
$$+\frac{y^4}{24}\left\{N^2c^3+A_2e^{\beta x}+A_1\beta^2xe^{\beta x}\left[\beta M+c(2p-N)+\beta\frac{cx}{2}(p-N)\right]\right\} \quad (36)$$

where A_1 and A_2 are integration constants.

For flows which are very near equilibrium, β is very large and negative. Thus neglecting the exponential terms in β, one has

$$\varphi(x,y) \approx c\,x^2/2 + y^2/2 \left\{ (N-P)c^2/\beta - Mc + Nc^2x \right\} + N^2c^3y^4/24 \qquad (37)$$

$$\varphi_x = cx + Nc^2y^2/2 , \qquad (38)$$

$$\varphi_y = y \left\{ (N-P)c^2/\beta - Mc + Nc^2x \right\} + N^2c^3y^3/6 \qquad (39)$$

Since the y component of the velocity is of higher order than the x component, the curves of constant velocity $q \approx a_f^* + \varphi_x$ are seen to be parabolic. Thus the initial data curve for supersonic flow computations by the method of characteristics can be taken as a parabolic arc with constant flow properties on this curve. The partially frozen sonic line and the curve of horizontal velocity are given by $\varphi_x = \varphi_y = 0$, respectively,

$$\text{Sonic line:} \qquad 0 = x + Ncy^2/2 \qquad (40)$$

$$\text{Horizontal velocity curve:} \quad 0 = x - \frac{M}{Nc}(1 + Pc/\beta) + Ncy^2/6 \qquad (41)$$

Eqs. (40), (41) show that these two curves do not meet on the axis as they do in perfect gas flows. The point where the line of horizontal velocity meets the x axis is given by

$$x^* = \frac{M}{Nc}(1 + Pc/\beta) \qquad (42)$$

It will be seen that x^* is upstream of the sonic point since M is negative. The displacement of the sonic point from the geometric throat is obtained by noting that $\varphi_y = 0$ for $y = H_0$ and $x = x_T$. Thus

$$x_T = \frac{M}{Nc}(1 + Pc/\beta) - NcH_0^2/6 = x^* - NcH_0^2/6 \qquad (43)$$

where x_T is the abscissa of the throat and H_o is the height at the throat. If the sonic line and line of horizontal velocity cross, this crossover point is given by the solution of Eqs. (40) and (41) for x, y. This point is,

$$x_c = (3M/2Nc)(1+Pc/\beta) = 3x^*/2$$
$$y_c = \left[-3M(1+Pc/\beta)\right]^{1/2}/Nc = (-3x^*/Nc)^{1/2} \qquad (44)$$

Limiting characteristics:

For reacting gas flows, the characteristics are the frozen Mach lines and their slopes are given as (in this case partially frozen characteristics)

$$dy/dx = \tan(\theta \pm \mu) \qquad (45)$$

where θ is the flow angle and μ is the Mach angle defined by $\sin\mu = 1/M_f$. In the sonic region, if the nozzle contour is sufficiently smooth and slowly varying, θ will be small compared to μ and hence using Eq. 22 one may approximate the characteristic directions by

$$dy/dx \approx \pm \tan\mu = \pm(M_f^2 - 1)^{-1/2} = \pm(P\varphi_x)^{-1/2} \qquad (46)$$

By using the solution for φ_x obtained earlier (Eq. (38)), Eq. (46) can be integrated to obtain the characteristic curves.

The characteristic which meets the sonic line on the axis divides the supersonic flow into two regions: I. that region wherein the characteristics emanating from the wall reflect on the sonic line and thus could affect the subsonic region and II. the purely supersonic region, which does not affect the subsonic region. The two characteristics that pass through the sonic point on the axis are given by

$$x - (Pcy^2/8)\left[1 \pm (1 + 8N/P)^{1/2}\right] = 0 \qquad (47)$$

It will be seen that these are parabolic. The point on the nozzle wall through which the limiting characteristic passes can be obtained by solving the wall equation

$$y = y_w(x) \tag{48}$$

and the left running characteristic equation

$$8x - Pcy^2 \left[1 - (1 + 8N/P)^{1/2}\right] = 0 \tag{49}$$

As an illustration, the flow of pure dissociated oxygen through a parabolic nozzle with reservoir conditions $T_o = 5900^oK$ and $p_o = 82$ atm. is calculated for a case for which quasi-one dimensional results were available. The results are presented in Fig. 1. The reference state values and the constant c in Eq. (35) were obtained from the quasi-one dimensional results.

It appears from a rough analysis that even if vibrational nonequilibrium were taken into account, the qualitative picture of the flow field would be very similar with the fully frozen Mach number replacing the partially frozen Mach number of the present note.

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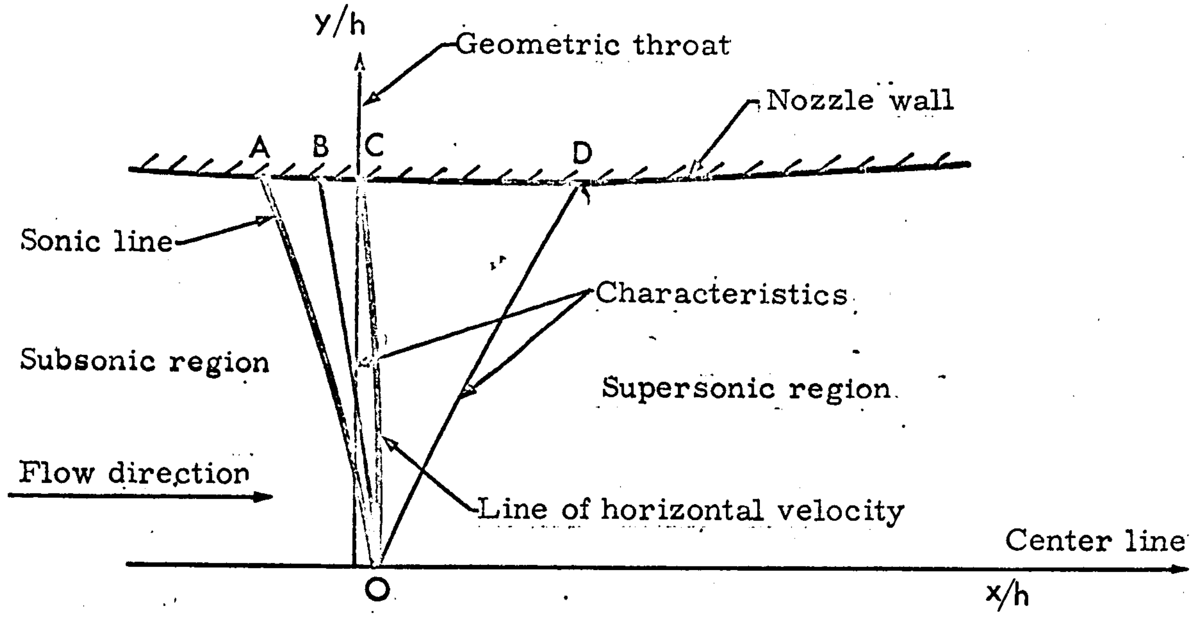
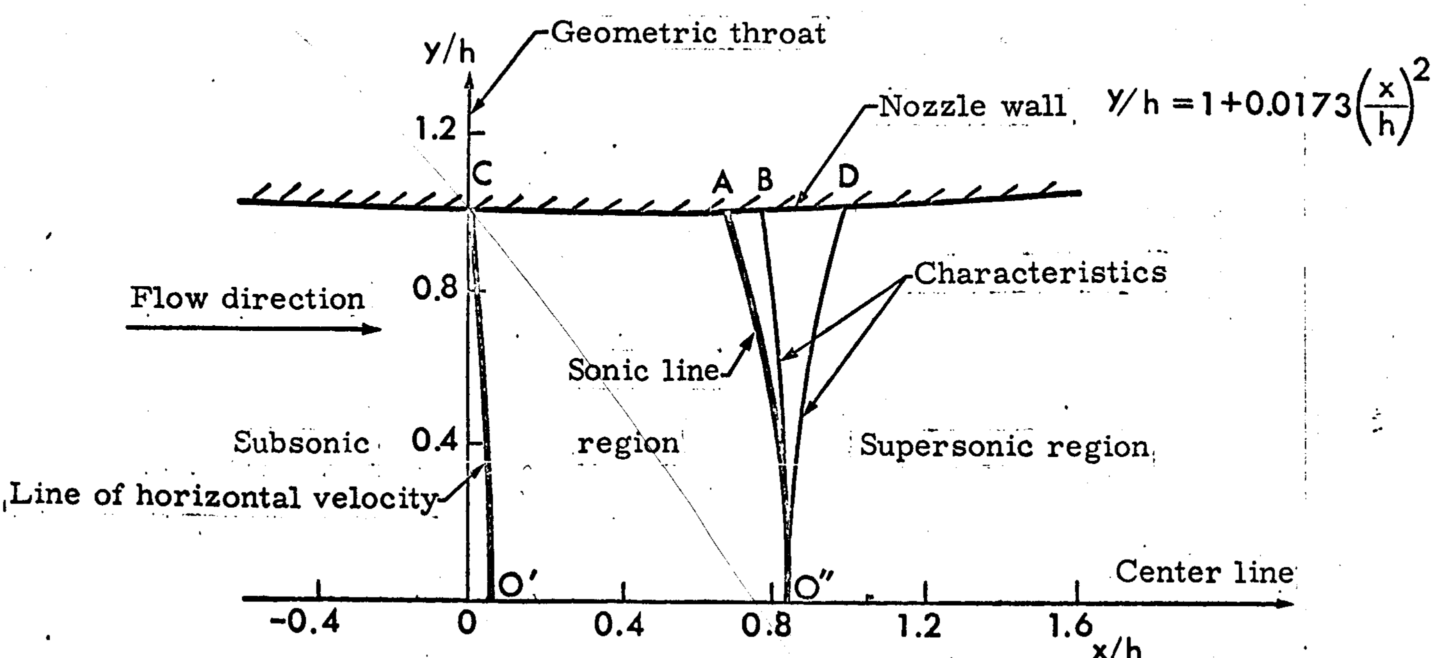


PERFECT GAS FLOW



REACTING GAS FLOW

Figure 1

NOZZLE TRANSONIC FLOW REGION IN A PERFECT GAS AND IN A DISSOCIATED OXYGEN FLOW

p_0=82atm., T_0=5900°K, α_0=0.69