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Technical Report

A HYDRODYNAMIC THEORY FOR THE INTERACTION OF A DETONATION WITH A COMPRESSIBLE BOUNDARY

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ABSTRACT

Detonations through an explosive of finite width are curved and propagate at a lower velocity than an ideal one-dimensional plane wave. A theory relating the velocity decrement and curvature of a gaseous detonation to the conditions at the explosive inert interface is developed. A two-dimensional detonation bounded on one side by a solid wall and on the other by an inert gas is considered. Approximate reaction zone equations are derived by expanding the flow variables in powers of a small parameter proportional to the ratio of reaction zone thickness to radius of curvature. Locally the reaction zone equations are the same as for one-dimensional flow with increasing area and heat addition, the rate of increase depending on the local wave curvature and the density variation through a plane detonation. Using Fay's result that the relative detonation velocity decrease is proportional to the fractional increase in the reaction zone streamtube area, an ordinary differential equation for variation of the wave angle is developed. Approximate solutions of the above equation yielded velocity decrements which agreed with experimental results.

I. INTRODUCTION

Detonations traveling through an explosive medium of finite width are curved and propagate at a lower velocity than an ideal one-dimensional plane wave. Since the extent of this effect, which is a result of the interaction between the detonation and the inert material bounding the explosive, depends upon the wave structure and thickness it has, in recent years, been the subject of a number of theoretical investigations attempting to relate measured velocity decrements to details of detonation structure. The present paper presents an analysis of detonations propagating through finite gaseous explosives, which hopefully avoids some of the difficulties of earlier theories.

It is generally agreed that the loss in velocity and the curvature of the wave are caused by the divergence of the streamlines within the reaction zone. The extent of this divergence depends upon the nature of the refraction at the interface between the explosive and the inert bounding material. In solid explosives conditions at the interface depend upon whether the charge is uncased or cased and on whether the case is thick or thin; for gaseous explosives the acoustic impedance of the inert relative to the explosive gas appears to be the determining factor. In the present paper we are concerned with gaseous explosives bounded by an infinite region of inert gas, which, as Sommers[1] has pointed out*, is analogous to a solid explosive with a very thick case.

One of the earliest treatments of the finite charge problem is due to Jones[2,3]. Rather than computing the details of the diverging flow within the reaction zone Jones ignored the curvature of the wave and approximated the reaction zone by

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*Numbers refer to the bibliography at the end of the paper.

an inner region of one-dimensional diverging flow. The actual expansion within the reaction zone is approximated by reaction products expanding through a Prandtl-Meyer wave at the outer edge of the region of one-dimensional flow, the streamline separating the two regions being determined by a pressure matching condition. The situation is shown in Fig. 1, which also shows the oblique shock induced in the boundary by the expanding charge. The Jones theory thus ignores wave curvature and must therefore depend on a theoretical model which is far removed from the actual conditions within the reaction zone of the curved detonation.

Eyring et al.[3], in their treatment of the problem took wave curvature into account and computed the wave shape in a finite cylindrical charge by replacing the curved detonation by a series of spherical detonation segments. It is shown that the divergence of the flow within the reaction zone, which is also responsible for the decrease in detonation velocity, depends upon the ratio of reaction zone thickness to the radius of curvature. The curvature of each wave segment is chosen so that the reduced detonation velocity equals the normal component of the oncoming flow. The detonation angle at the edge of the charge is established by requiring the flow angle and pressure behind the detonation and behind the oblique shock which propagates into the case to be equal. In the theory of Eyring et al., it is assumed that the flow is steady relative to the spherical detonation segments, which is self-contradictory since spherical detonations are inherently unsteady[4]. Since it is the flow within the reaction zone which determines the wave curvature and velocity, it also appears inconsistent to use conditions behind the detonation to establish the interface boundary condition.

Wood and Kirkwood[5] determined the effect of wave curvature upon the propagation velocity of steady detonations in an analysis which was based upon the inviscid conservation equations applied to the reaction zone. However, their analysis did not consider the finite charge problem and so they do not establish any relation between the curvature of the wave and the conditions at the explosive inert interface.

Both from an experimental and theoretical standpoint gaseous detonations are much simpler to study than detonations[5] in solid and liquid explosives, and this fact provided the impetus for the experimental investigation of gaseous detonations in the presence of inert compressible boundaries by Sommers[1] and Dabora[6]. To explain his results Dabora used a one-dimensional theory similar to that of Jones; however, rather than introducing the artificial concept of an outer Prandtl-Meyer expansion the flow divergence within the one-dimensional reaction zone is determined by matching the flow behind the detonation to that behind the oblique shock in the inert boundary as in the theory of Eyring et al.[3].

The curved front theory developed below is closely related to that of Wood and Kirkwood[5] in that the inviscid conservation equations of the reaction zone provide the starting point. In contrast to the theories above conditions within the reaction zone are employed to establish the nature of the wave refraction at the explosive-inert interface.

II. FORMULATION OF FIRST ORDER REACTION ZONE EQUATIONS

A two-dimensional detonation propagating with velocity D through an explosive gas of width L bounded on one side by a solid wall and on the other by an inert gas is considered. The above corresponds to the configuration investigated experimentally by Dabora[6] and is shown schematically in Fig. 2(a) from the point of view of an observer fixed to the wave while Fig. 2(b) shows a typical Schlieren picture of such a wave as obtained by Dabora. The analysis is based on the Von-Neumann-Döring model of detonation structure in which the wave is treated as a shock of infinitesimal thickness followed by an inviscid reaction zone.

As in the analysis of curved shock wave structure[7,8] shock based coordinates, as shown in Fig. 3, appear to be the most natural ones to use for the equations describing the flow within the reaction zone. In this coordinate system the continuity equation and the momentum equations along and normal to the detonation are

$$\frac{\partial (\rho u)}{\partial x} + (1 - Ky) \frac{\partial (\rho v)}{\partial y} - K\rho v = 0 \tag{1}$$

$$u \frac{\partial u}{\partial x} + (1 - Ky) v \frac{\partial u}{\partial y} - Kuv + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0 \tag{2}$$

$$u \frac{\partial v}{\partial x} + (1 - Ky) v \frac{\partial v}{\partial y} + Ku^2 + \frac{(1 - Ky)}{\rho} \frac{\partial p}{\partial y} = 0 \tag{3}$$

where x and y and the corresponding velocities u and v are along and normal to the wave respectively.

$$K = \text{curvature} = \frac{1}{R} = \frac{d\alpha}{dx} \tag{4}$$

where α is the wave angle defined in Fig. 3.

In the absence of viscous dissipation and conduction the energy equation is simply

$$h + \frac{u^2}{2} + \frac{v^2}{2} = h_o = \text{const} \tag{5}$$

where now h includes the heats of formation of the chemical species present within the reaction zone.

In addition to the above, the chemical kinetic equations, and a thermodynamic equation of state are required to completely specify conditions within the reaction zone. Following the notation of Wood and Kirkwood[9] the stoichiometric equation for each chemical reaction is written in the form

$$\sum_s \nu_s^{\alpha} X_s = 0 \quad , \quad (\alpha = 1, 2 \ldots n) \tag{6}$$

where X_s represents a unit mass of species s and ν_s^{α} is the specific stoichiometric coefficient for species s in the αth reaction. Defining a progress variable, λ_{α}, for the αth reaction by

$$d\kappa_s = \sum_{\alpha} \nu_s^{\alpha} d\lambda_{\alpha} \quad , \quad (\alpha = 1, \ldots n) \tag{7}$$

where κ_s is the mass fraction of species s the reaction rates are given by

$$\frac{d\lambda_{\alpha}}{dt} = r_{\alpha} \tag{8}$$

where r_{α}, the rate of the αth reaction, is taken as a function of the local thermodynamic variables. In shock based coordinates the Lagrangian derivative d/dt is given by

$$\frac{d}{dt}(\ ) = u\frac{\partial}{\partial x}(\ ) + (1 - Ky)\, v\frac{\partial}{\partial y}(\ ) \tag{9}$$

Assuming that thermodynamic quasi-equilibrium exists, i. e. , thermal and mechanical equilibrium but not chemical equilibrium, it is possible to use the usual thermodynamic equations of state with the λ_α as additional independent variables. All thermodynamic variables can, for example, be expressed as functions of T, ρ and the progress variables λ_α.

If there are n reactions then with the equation of state there are n + 5 independent equations for the n + 7 variables λ_α, ρ, u, p, v, K, D, and h, so that the number of unknowns exceeds the number of equations by two. Only one extra unknown, the propagation velocity D, appears in the formulation of the plane detonation equations, and its value is determined by the introduction of the Chapman-Jouguet (C-J) condition. Now the curvature K(x) enters as an additional variable and its evaluation must in some way be related to conditions where the detonation meets the inert boundary gas. Essentially the variation of K(x) must be consistent with the refraction at the explosive-inert interface. Furthermore, the propagation velocity D and the curvature K(x) are not independent of each other, an increase in K(x) generally resulting in a reduction in D. Exact solution of the curved front problem formulated above presents formidable difficulties; however, since the relative decrease in D due to curvature, and $K\ell_o$ the ratio of a characteristic reaction zone length ℓ_o to shock radius of curvature R are usually small approximate solution of the problem becomes possible. In H_2 - O_2 detonations for example reduction of the plane wave velocity by more than about 10% generally results in quenching[6].

The basic equations above are supplemented by the following reactive flow relation between pressure and density as derived by Kirkwood and Wood[12]:

$$\frac{d\rho}{dt} = \frac{1}{c_o^2}\frac{dp}{dt} - \rho \sum_\alpha \sigma_\alpha r_\alpha \tag{10}$$

where C_o is the frozen sound speed,

$$\sigma_\alpha = \frac{\rho\beta^o}{C_p^{\ o}}\left(\frac{C_p^{\ o}\Delta_\alpha v}{\beta_o} - \Delta_\alpha h\right)$$

$C_p^{\ o}$ is the frozen constant pressure specific heat, v is the specific volume, β_o is the frozen expansion coefficient given by

$$\beta_o = \left(\frac{\partial v}{\partial T}\right)_{p,\{\lambda\}}$$

while the operator Δ_α is defined as

$$\Delta_\alpha = \frac{\partial}{\partial\lambda_\alpha}(\ )_{T,p,\{\lambda_\alpha\}} \quad .$$

The subscript λ signifies that all progress variables are held constant while λ_α signifies that all progress variables except λ_α are held constant.

The present situation is similar to the problem of finding the influence of shock wave curvature and thickness upon the Hugoniot conditions, as considered for example by Probstein and Pan[7], and Germain and Guiraud[8]. In the case of the detonation both the effects of reaction zone thickness and the variation of the wave angle α must be considered. To evaluate the thickness effect it is convenient to follow a procedure similar to that of Germain and Guiraud. The coordinates x and y are stretched according to

$$d\bar{x} = \frac{dx}{R(x)} \quad ; \quad \bar{y} = \frac{y}{\ell_o} \tag{11}$$

so that significant changes in x and y will be of the same order of magnitude within the reaction zone. With the introduction of these stretched coordinates the continuity, and the momentum equations become

$$\delta \frac{\partial(\rho u)}{\partial \overline{x}} + (1 - \delta\overline{y}) \frac{\partial(\rho v)}{\partial \overline{y}} - \delta\rho v = 0 \tag{12}$$

$$\delta u \frac{\partial u}{\partial \overline{x}} + (1 - \delta\overline{y})\, v \frac{\partial u}{\partial \overline{y}} - \delta u v + \frac{\delta}{\rho}\frac{\partial p}{\partial \overline{x}} = 0 \tag{13}$$

$$\delta u \frac{\partial v}{\partial \overline{x}} + (1 - \delta\overline{y})\, v \frac{\partial v}{\partial \overline{y}} + \delta u^2 + \frac{(1 - \delta\overline{y})}{\rho}\frac{\partial p}{\partial \overline{y}} = 0 \tag{14}$$

where $\delta = \frac{\ell_o}{R}$,

and usually, $\delta << 1$.

Now as in Refs. 7 and 8 it is assumed that the variables within the reaction zone may be expanded in the small parameter δ so that

$$\begin{aligned}
u &= u^{(0)} + \delta u^{(1)} + 0(\delta^2)\\
v &= v^{(0)} + \delta v^{(1)} + 0(\delta^2)\\
\rho &= \rho^{(0)} + \delta\rho^{(1)} + 0(\delta^2)\\
\rho v &= (\rho v)^{(0)} + \delta(\rho v)^{(1)} + 0(\delta^2)\\
p + \rho v^2 &= (p + \rho v^2)^{(0)} + \delta(p + \rho v^2)^{(1)} + 0(\delta^2)\\
\lambda &= \lambda^{(0)} + \delta\lambda^{(1)} + 0(\delta^2)
\end{aligned} \tag{15}$$

In Eq. (15) the zeroth order terms represent the plane wave solution for which $\delta = 0$. Since in a plane wave

$$\frac{\partial u^{(0)}}{\partial \overline{y}} = \frac{\partial(\rho v)^{(0)}}{\partial \overline{y}} = \frac{\partial}{\partial \overline{y}}(p + \rho v^2)^{(0)} = 0 \tag{16}$$

introduction of (15) in the continuity and momentum Eqs. (12)-(14) leads to the equations

$$\frac{\partial(\rho v)}{\partial \bar{y}} = \delta\left[(\rho v)^{(0)} - u^{(0)}\frac{\partial \rho^{(0)}}{\partial \bar{x}} - \rho^{(0)}\frac{\partial u^{(0)}}{\partial \bar{x}}\right] + 0(\delta^2) \tag{17}$$

$$\frac{\partial u}{\partial \bar{y}} = \frac{\delta}{v^{(0)}}\left[u^{(0)}\, v^{(0)} - u^{(0)}\frac{\partial u^{(0)}}{\partial \bar{x}} - \frac{1}{\rho^{(0)}}\frac{\partial p^{(0)}}{\partial \bar{x}}\right] + 0(\delta^2) \tag{18}$$

$$\frac{\partial}{\partial \bar{y}}(\rho v^2 + p) = \delta\left[v^{(0)}\left\{(\rho v)^{(0)} - \rho^{(0)}\frac{\partial u^{(0)}}{\partial \bar{x}}\right\} - \rho^{(0)}\, {u^{(0)}}^2 - u^{(0)}\frac{\partial (\rho v)^{(0)}}{\partial \bar{x}}\right] \tag{19}$$

which show the effect of thickness and curvature on the variation of mass flow density ρv, tangential velocity u and total momentum $p + \rho v^2$, quantities which remain invariant across a plane wave. To $0(\delta)$ the above derivatives depend only upon the zeroth order or plane wave solution.

It is assumed that the expansions of Eq. (15) are uniform, or in other words that the ratios $u^{(1)}/u^{(0)}$, $v^{(1)}/v^{(0)}$, $\rho^{(1)}/\rho^{(0)}$, etc., are all of $0(1)$. It is of course, also possible to question whether or not the deviations from the plane detonation structure should be of $0(\delta)$ instead of say $0(\delta^{3/2})$ or $0(\delta^{1/2})$. From relations between the shock angle α and the streamline angle behind the shock[10] it is readily shown that the relative increase in streamtube area dA/A behind a curved shock wave varies as δ. Furthermore, in simple one-dimensional flows with a small relative area change, the resultant changes in pressure, temperature, velocity, and density all vary linearly with dA/A[11], so that the expansion in δ is certainly justified on physical grounds.

As will be seen later, it is convenient to write the energy equation in the form

$$\frac{\partial}{\partial \bar{y}}\left(h + \frac{v^2}{2}\right) = -\frac{\partial}{\partial \bar{y}}\left(\frac{u^2}{2}\right) = -\delta u^{(0)}\frac{\partial u^{(1)}}{\partial \bar{y}} \tag{20}$$

The magnitudes of the zeroth order quantities on the right of Eqs. (16-19) depend upon the magnitude of the angle α. Thus

$$u^{(0)} = D \sin \alpha \tag{21}$$

$$(\rho v)^{(0)} = \rho_{\infty} D \cos \alpha \tag{22}$$

while immediately behind the shock

$$\frac{\rho_1^{(0)}}{\rho_{\infty}} = \frac{(\gamma + 1) M_{\infty}^2}{(\gamma - 1) M_{\infty}^2 + \frac{2}{\cos^2 \alpha}} \tag{23}$$

$$\frac{p_1^{(0)}}{p_{\infty}} = \frac{2\gamma M_{\infty}^2 \cos^2 \alpha - (\gamma - 1)}{(\gamma + 1)} \ . \tag{24}$$

M_{∞} is the propagation Mach number of the detonation. As mentioned previously, D depends upon the wave curvature but if it is assumed that the deviation of D from the plane wave propagation velocity $D^{(0)}$ is $0(\delta)$ so that

$$D = D^{(0)} + \delta D^{(1)} \tag{25}$$

then $D^{(0)}$ can be used in the above expressions for the zero order quantities. The above assumption will be found to be consistent with the results to follow.

Introduction of Eqs. (21), (22), and (23) in Eq. (17) leads to the result

$$\frac{\partial}{\partial y}\left[\frac{\rho v}{\rho_{\infty} D^{(0)}}\right] = \delta \cos \alpha \left\{1 - \frac{\rho^{(0)}}{\rho_{\infty}} + 0\left[\frac{4(\gamma + 1)}{(\gamma - 1)^2 M_{\infty}^4} \tan^2 \alpha \sec^2 \alpha\right]\right\} , \tag{26}$$

In deriving the above equation the variation of α with respect to $\bar{x}$ has been taken into account so that for example

$$\frac{\partial u^{(0)}}{\partial \bar{x}} = \frac{\partial u^{(0)}}{\partial x} \frac{dx}{d\bar{x}} = D^{(0)} \cos \alpha \frac{d\alpha}{dx} \frac{dx}{d\bar{x}} = D^{(0)} \cos \alpha \ .$$

It has been assumed that the magnitude of $\partial\rho^{(0)}/\partial x$ at the shock, i. e., $\partial\rho_1^{(0)}/\partial x$ is representative of the magnitude of this quantity throughout the reaction zone. For $\alpha << 1$ and for the relatively large values of M_∞ typical of detonations the continuity equation (26) thus can be approximated by

$$\frac{\partial}{\partial \bar{y}}\left[\frac{\rho v}{\rho_\infty D^{(0)}}\right] = \delta\left(1 - \frac{\rho^{(0)}}{\rho_\infty}\right) \quad . \tag{27}$$

It should be noted that the quantity $(\rho v/\rho_\infty D^{(0)})$ within the brackets will be of 0(1) within the reaction zone. Similarly introduction of Eqs. (21)-(24) in the momentum and energy equations (18)-(20) leads to the results

$$\frac{\partial}{\partial \bar{y}}\left[\frac{u}{D^{(0)}\sin\alpha}\right] = \delta\left[1 - \frac{\rho^{(0)}}{\rho_\infty} + 0(1)\right] \tag{28}$$

$$\frac{\partial}{\partial \bar{y}}\left[\frac{\rho v^2 + p}{\rho_\infty D^{(0)^2}}\right] = \delta\left(\frac{\rho_\infty}{\rho^{(0)}}\right)\cos^2\alpha\left[\left(1 - \frac{\rho^{(0)}}{\rho_\infty}\right) - \frac{\rho^{(0)}}{\rho_\infty}\left(1 + \frac{\rho^{(0)}}{\rho_\infty}\right)\tan^2\alpha\right] \tag{29}$$

$$\frac{\partial}{\partial \bar{y}}\left[\frac{h + \frac{v^2}{2}}{\frac{D^{(0)^2}}{2}}\right] = 2\,\delta\sin^2\alpha\left[1 - \frac{\rho^{(0)}}{\rho_\infty} + 0(1)\right] \quad . \tag{30}$$

The quantities in brackets on the left side of the above equations are all 0(1) in the reaction zone. While the changes in $u/D^{(0)}\sin\alpha$, $(p + \rho v^2)/\rho_\infty D^{(0)2}$ are of order δ across the reaction zone the change in $(h + v^2/2)/D^{(0)2}/2$ will be of order $\delta\sin^2\alpha$, so that the energy equation reduces to

$$h + \frac{v^2}{2} = \text{const} \tag{31}$$

for $\alpha << 1$. From Eq. (31) the important result that the x momentum equation for u is uncoupled from the y momentum and energy equations follows. Clearly when $\alpha << 1$ the term with coefficient $\tan^2 \alpha$ can be dropped from Eq. (29).

The conservation equations fail to provide sufficient information for determining the propagation velocity of a detonation wave; however, it is found that unsupported plane waves propagate with a velocity such that the gases at the end of the reaction move with sonic velocity with respect to the wave, and this is the well known Chapman-Jouguet condition. Physically this result is justified by the argument that with sonic velocity behind the reaction zone downstream disturbances can no longer overtake the wave making steady propagation possible. If the reactions within the detonation are reversible both an equilibrium and a frozen speed of sound may be defined and then there is some ambiguity as to which sound speed to use in the Chapman-Jouguet condition. Recently Wood and Kirkwood[13], and Wood and Salsburg[14] have shown that the Chapman-Jouguet condition should be based on the equilibrium rather than the frozen speed of sound as previously suggested[12]. A simple physical argument for the plausibility of this conclusion[14] is based upon Chu's[15] result for near equilibrium flows that while the wave head of an unsteady rarefaction moves with the frozen speed of sound, the bulk of the disturbance will, after sufficient time has elapsed, move with the equilibrium speed of sound. Consequently the main disturbance of the rarefaction wave that usually follows the C-J detonation can never overtake the detonation even when the equilibrium speed of sound is used to formulate the C-J condition.

In the model under consideration here the curved detonation is followed by a steady Prandtl-Meyer expansion rather than by an unsteady rarefaction wave. Furthermore, stream tube area varies through and behind the wave due to the curvature effects. Consequently the nature of the curved wave Chapman-Jouguet condition is unclear, for the arguments used to establish the nature of the C-J condition no longer apply. In attempting to establish the conditions to be satisfied at the downstream edge of the reaction zone it is useful to eliminate the derivatives of pressure and density by combining the momentum and continuity equations (12)-(14) with Eq. (10) relating to $d\rho/dt$ to dp/dt, with the resulting equation

$$\delta\left(1 - \frac{u^2}{c_o^2}\right)\frac{\partial u}{\partial \bar{x}} + (1 - \delta\bar{y})\left(1 - \frac{v^2}{c_o^2}\right)\frac{\partial v}{\partial \bar{y}} - \frac{uv}{c_o^2}\left[(1 - \delta\bar{y})\frac{\partial u}{\partial \bar{y}} + \delta\frac{\partial v}{\partial \bar{x}}\right] =$$

$$\delta v + \sum_\alpha \sigma_\alpha\left[\delta u\frac{\partial \lambda_\alpha}{\partial \bar{x}} + (1 - \delta\bar{y})\, v\frac{\partial \lambda_\alpha}{\partial \bar{y}}\right] \qquad (32)$$

Equation (32) is the reactive form of the "gas dynamic" equation of compressible flow. Introducing the expansions (15) and Eqs. (21)-(24) and dropping terms of $0(\delta \sin^2 \alpha)$ as well as replacing $(1 - \delta\bar{y})$ by 1.0 Eq. (32) reduces to

$$\left(1 - \frac{v^2}{c_o^2}\right)\frac{\partial v}{\partial \bar{y}} = -\delta v^{(0)}\left(\frac{\rho^{(0)}}{\rho_\infty} - 1\right) + \sum_\alpha \sigma_\alpha v^{(0)}\frac{\partial \lambda_\alpha^{(0)}}{\partial \bar{y}} \qquad (33)$$

where for the present we have not expanded the left side of Eq. (33). For convenience in the discussion below the abbreviations

$$\mathcal{D} = \delta v^{(0)}\left(\frac{\rho^{(0)}}{\rho_\infty} - 1\right) = \delta\left(D^{(0)} - v^{(0)}\right)$$

$$\mathcal{R} = \sum_\alpha \sigma_\alpha v^{(0)}\frac{\partial \lambda_\alpha^{(0)}}{\partial \bar{y}} \qquad (34)$$

are introduced. It is readily shown that $\mathcal{D}$, which represents the effect of stream-tube divergence due to detonation curvature is always positive and decreases with increasing $\bar{y}$. $\mathcal{R}$ represents the effect of chemical reaction upon the velocity v.

In a plane wave $\mathscr{D} = 0$. At the C-J point $v = c$, where c is the equilibrium speed of sound. Since $c \leq c_o$, always[14] it follows that $(1 - c^2/c_o^2) \geq 0$ and at the equilibrium C-J point it follows that since $\partial\lambda_\alpha/\partial\bar{y} = 0$, $\partial v/\partial\bar{y} = 0$. Thus the plane wave equilibrium C-J point occurs at $\bar{y} \to \infty$ where all variations have disappeared. If it is assumed that v always approaches c monotonically, an assumption which is supported by the reaction profile calculations of Duff[16], then $\mathscr{R} \geq 0$ in the reaction zone; however, it is difficult to arrive at general conclusions regarding the behavior of $\mathscr{R}$. In a curved detonation the divergence term $\mathscr{D}$ opposes the accelerating effect of the chemical reaction term and results in a reduction in the velocity gradient $\partial v/\partial\bar{y}$, at least for $v < c_o$. The velocity variation within the reaction zone of the curved wave will depend upon the relative magnitudes of $\mathscr{R}$ and $\mathscr{D}$ and upon whether $(1 - v^2/c_o^2)$ is positive or negative. Several possible conditions at the edge of the reaction zone will now be considered.

Within the reaction zone itself $\mathscr{R} > \mathscr{D}$ so that v accelerates from the subsonic value immediately behind the shock, and it is presumed that v ultimately will reach the equilibrium sonic speed c. If when first $v = c$, $\mathscr{R} = 0$ so that $(\mathscr{R} - \mathscr{D}) < 0$, it follows than then $(\partial v/\partial\bar{y}) < 0$ implying a velocity maximum $v_{max} > c$ at some point upstream which contradicts the fact that the point where v first reaches c is under consideration. Hence $(\mathscr{R} - \mathscr{D}) \geq 0$ when $v = c$. If $(\mathscr{R} - \mathscr{D}) = 0$, $\partial v/\partial\bar{y} = 0$ and v has a maximum or inflection point. If $\mathscr{R}$ decreases with increasing $\bar{y}$ such that $(\mathscr{R} - \mathscr{D}) < 0$, v decreases below c, a result which is at variance with continued increase of v through the Prandtl-Meyer wave behind the reaction zone, though it is not entirely inconceivable that there is a region in which v passes through several maxima and minima. Of course another possibility is that $(\mathscr{R} - \mathscr{D})$ remains at zero with increasing $\bar{y}$. Such a condition implies $v = \text{const} = c$ and $\mathscr{D} = \text{const}$. However since $\mathscr{R} > 0$ for $(\mathscr{R} - \mathscr{D}) = 0$ chemical reactions must be occurring tending toward chemical equilibrium, which is at variance with the requirement that $\mathscr{R} = \text{const} = \mathscr{D}$. Physically the most plausible condition is that $(\mathscr{R} - \mathscr{D}) > 0$ when $v = c$. The assumption that the velocity continues to increase monotonically throughout the reaction zone finally leads to the requirement that $(\mathcal{R} - \mathcal{D}) = 0$ when $v = c_o$, and this corresponds to the modified C-J condition used by Eyring[3], and by Wood and Kirkwood[6] in their curved front theories. In some sense it may be more meaningful to refer to this condition as the curved wave choking condition rather than as a C-J condition.

In the model under consideration here a Prandtl-Meyer expansion propagates into the explosive from the edge of the wave as shown in Figs. 2a, and 4. It has been shown[23,24] that near the vertex of a P-M (Prandtl-Meyer) expansion fan the bulk of the disturbance lies along the frozen wave fronts and this fact lends further support to the use of the curved wave choking condition above. An important unanswered question, and one which was also asked by Wood and Salsburg[14], is how does the transition from the curved wave choking condition to the equilibrium C-J condition occur as the wave radius of curvature R approaches infinity.

In order to close the first order curved reaction zone equations above it becomes necessary to in some way introduce the conditions at the explosive inert interface. To this end the first order equations above will be used to derive a differential equation for the variation of the wave angle α with the position x along the wave.

The conservation equations (27)-(30) are readily integrated with respect to $\bar{y}$. With the introduction of the function $\mathcal{L}(\bar{y}, x)$ defined by

$$\mathcal{L}(\bar{y}, \bar{x}) = \delta \int_0^{\bar{y}} \left(\frac{\rho^{(0)}}{\rho_\infty} - 1 \right) d\bar{y} \tag{35}$$

and letting ℓ be the reaction zone thickness, the integrated first order conservation equations become

$$(\rho v)_1 = (\rho v)_2 \left[1 + \mathcal{L}\left(\frac{\ell}{\ell_o} \right) \right] \tag{36}$$

$$u_1 = u_2 \left[1 + \mathcal{L}\left(\frac{\ell}{\ell_o}\right)\right] \tag{37}$$

$$(\rho v^2 + p)_1 = (\rho v^2 + p)_2 \left[1 + \mathcal{L}\left(\frac{\ell}{\ell_o}\right)\right] + \int_0^{\frac{\ell}{\ell_o}} p^{(0)} \frac{\partial \mathcal{L}}{\partial \bar{y}} d\bar{y} \tag{38}$$

In deriving these equations the assumption that $\alpha << 1$ has been used as well as the fact that to first order

$$(\rho v) \cong \rho_\infty D^{(0)} \quad , \quad u_1 \cong D^{(0)} \sin \alpha$$

$$(\rho v^2 + p)_1 \cong \left(\rho^{(0)} {v^{(0)}}^2 + p^{(0)}\right) .$$

The first order C-J or, perhaps more appropriately, choking condition becomes

$$\left.\frac{\partial \mathcal{L}}{\partial \bar{y}}\right|_{\bar{y}=\frac{\ell}{\ell_o}} = \sum_\alpha \sigma_\alpha \left.\frac{\partial \lambda_\alpha^{(0)}}{\partial \bar{y}}\right|_{\bar{y}=\frac{\ell}{\ell_o}} \tag{39a}$$

$$v = c_o . \tag{39b}$$

The formulation of the first order curved detonation equations is essentially complete for the conservation equations (31), (36), and (38) together with the C-J condition (39), the rate equation (8) and an appropriate equation of state are sufficient to determine the component of D normal to the wave front provided that the radius of curvature R(x) is known. Clearly, then, the problem of relating R(x) to boundary conditions at the edge of the wave remains, and is considered in the section which follows.

For fixed x equations (31), (36), (38), and (39) have the same form as the one-dimensional reaction zone equations used by Fay[17] in his analysis of the effect of the boundary layer upon the velocity of detonations in tubes. In the one-dimensional case $d\mathcal{L}$ equals the fractional streamtube area increase dA/A. In the present curved front case the differential $d\mathcal{L}$ can be assigned a similar interpretation. Hayes and Probstein[10] show that behind any curved hydrodynamic discontinuity with density ratio ρ_s/ρ_∞, and such that the tangential component of velocity is conserved, the streamline angle θ_s and the shock or discontinuity angle α are related by

$$\frac{d\theta_s}{d\alpha} = \left(\frac{\rho_s}{\rho_\infty} - 1\right) \tag{40}$$

at the point where $\alpha = 0$, i. e., where the discontinuity is normal to the oncoming flow. Consequently for a streamtube behind such a discontinuity

$$\frac{dA}{A} = \frac{d\theta_s dy}{R d\alpha} = \frac{\ell_o}{R}\left(\frac{\rho_s}{\rho_\infty} - 1\right) d\bar{y} \tag{41}$$

Comparing Eqs. (35), and (41) it is clear that $d\mathcal{L}$ represents the local value of dA/A within the reaction zone of the detonation subject to the assumption $\alpha << 1$. Equations (35), (36), (38), and (31) thus indicate that for a fixed value of x the flow behaves as a one-dimensional flow with variable area, the area increase being a function of the local curvature and the density profile through the reaction zone. This one-dimensional character of the curved front flow provides the basis for the approximate solution developed below. As mentioned before, the tangential momentum equation is completely uncoupled from the other equations to the present order of approximation.

III. THE VELOCITY DECREMENT AND WAVE SHAPE

It has been shown above that to first order in δ the curved front reaction zone equations are identical to the equations for one-dimensional flow with variable area used by Fay[17] in his analysis of the boundary layer induced velocity decrement of detonations in tubes. From numerical solutions of these equations Fay found that for $\mathcal{L} << 1$ the relation

$$\frac{D^{(0)} - D \cos \alpha}{D^{(0)}} = K_1 \, \epsilon \mathcal{L}\left(\frac{\ell}{\ell_o}\right) \tag{42}$$

is valid to an accuracy of a few percent. In (42) K_1 is a constant, $D \cos \alpha$ is the component of propagation velocity normal to the wave, and ϵ is related to the integral in equation (38) by

$$\int_0^{\frac{\ell}{\ell_o}} p^{(0)} \frac{\partial \mathcal{L}}{\partial \bar{y}} d\bar{y} = p_2^{(0)} \mathcal{L}\left(\frac{\ell}{\ell_o}\right) \epsilon \tag{43}$$

where

$$1 \leq \epsilon \leq 2 \quad .$$

Wood and Kirkwood[5] arrived at a similar result in their curved front analysis. Fay's result will be used directly below for the object of the present analysis is not so much to compute the exact effect of curvature upon local velocity decrement as to establish how boundary conditions at the explosive-inert interface affect propagation.

Introducing the definition of $\mathcal{L}$ into equation (42) now yields the following differential equation for the wave angle α as a function of x

$$1 - (1 - \eta) \cos \alpha = K_1 \epsilon \ell_o \frac{d\alpha}{dx} \Lambda \tag{44}$$

where

$$\eta = \frac{D^{(0)} - D}{D^{(0)}} \quad , \quad \Lambda = \int_0^{\frac{\ell}{\ell_o}} \left(\frac{\rho^{(0)}}{\rho_\infty} - 1 \right) d\bar{y} \quad .$$

In general both the reaction zone thickness ℓ, and hence Λ, are functions of x, the distance along the wave. It is necessary to use the choking condition as expressed by Eq. (39a) to determine the variation of the reaction zone thickness ℓ, and in view of Eq. (44) this equation can be written in the form

$$\frac{1 - (1 - \eta) \cos \alpha}{K_1 \epsilon \Lambda} \left[\frac{\partial}{\partial \bar{y}} \int_0^{\bar{y}} \left(\frac{\rho^{(0)}}{\rho_\infty} - 1 \right) d\bar{y} \right]_{y = \frac{\ell}{\ell_o}} = \sum \sigma_\alpha \frac{\partial \lambda_\alpha^{(0)}}{\partial \bar{y}} \quad . \tag{45}$$

An approximate form of the conditions $v = c_o$ has already been used by Fay in arriving at Eq. (42).

It now becomes expedient to let ℓ_o equal the reaction zone thickness at $x = 0$ where the wave front is normal to the oncoming flow. If now it is assumed that along the wave $\Delta\ell/\ell_o << 1$ so that approximately $\ell/\ell_o = 1$, then Eqs. (44) and (45) reduce to relatively simple simultaneous ordinary differential equations for ℓ_o and $\alpha(x)$. Equation (45) can be used to show that

$$\frac{\Delta \ell}{\ell_o} \sim 0 \left(\alpha \eta \frac{L}{\ell_o} \right)$$

provided a one step reaction model in which λ approaches its equilibrium value exponentially is used to evaluate the reaction rate term.

The wave angle Eq. (44) can be integrated in analytical form and upon introducing the boundary condition $\alpha = 0$ when $x = 0$, which implies negligible wall boundary layer effects, the following relation between α and x is obtained:

$$\tan \frac{\alpha}{2} = \sqrt{\frac{\eta}{2 - \eta}} \tan \frac{x}{\ell_o} \frac{\sqrt{\eta}\,(2 - \eta)}{2K_1 \epsilon \Lambda} \tag{46}$$

The dimensionless velocity decrement η plays the role of an eigenvalue in Eq. (46), its value being determined by the interface boundary condition $\alpha = \alpha_i$ at $x = x_i$. Since $x_i \cong L$ to quantities of higher order in the present case, the velocity decrement η is determined by the equation

$$\tan \frac{\alpha_i}{2} = \sqrt{\frac{\eta}{2 - \eta}} \tan \frac{L}{\ell_o} \frac{\sqrt{\eta}\,(2 - \eta)}{2K_1 \epsilon \Lambda} \quad . \tag{47}$$

Equations (46) and (47) now provide the desired link between the wave shape, the velocity decrement, and the conditions at the explosive-inert interface. In order to determine α_i, the nature of the flow at the explosive-inert interface must be studied in detail.

The interaction at this interface, particularly at the point where the shock preceeding the reaction zone meets the inert gas, is closely related to the refraction of an ordinary hydrodynamic shock, by a surface of separation between two gases. If the angle between the interface and the incident shock, ($\pi/2 - \alpha$ in the present notation) is sufficiently small a shock is transmitted across the interface and either a shock wave or an expansion wave is reflected from the interface. The theory of such "regular" refractions is well understood[18] and has been verified by experimental observations[19]. Whether the reflected wave is an expansion or compression depends upon the strength of the incident wave and the values of γ and the speed of sound in the two adjacent gases.

As the angle between the incident shock and the interface increases beyond some critical value, the simple configuration described above no longer can satisfy all the deflection and pressure conditions at the interface. The flow, which then is called an irregular refraction, becomes very complex, and though extensive experimental observations of irregular refractions were made by Jahn[19], no adequate theory is available. The nature of the interaction then depends drastically upon the relative values of the speed of sound and the ratio of specific heats on the two sides of the interface.

The interaction process under consideration here falls into the class of irregular refractions since the angle between the detonation and the interface is always very close to 90^{o}. The experiments of Dabora[6] and Sommers[1] show that the nature of the refraction depends in a crucial way upon whether the acoustic impedance, ρa, of the inert gas is greater or less than the acoustic impedance of the unreacted explosive, or more precisely, the refraction depends upon the acoustic impedance ratio $(\rho_5 a_5)/(\rho_\infty a_\infty)$. Subscripts ∞ and 5 refer to the explosive and inert gases respectively. When $\gamma_\infty = \gamma_5$ and $p_\infty = p_5$ the impedance ratio reduces to, (a_∞/a_5), the ratio of sonic velocities in the two media.

When $a_5 < a_\infty$ the refraction is relatively simple for then an oblique shock with supersonic velocity behind it is usually transmitted into the inert gas, and it is this situation which will be considered in detail below. On the other hand when $a_5 > a_\infty$ complicated interaction patterns result, and in some cases both Dabora[6] and Jahn[19] have observed transmitted waves which actually precede the incident detonation or shock.

The flow at the inert-explosive interface must adjust itself to contain the high pressure behind the shock and within the reaction zone relative to the low pressure in the inert bounding gas. When $a_5 < a_\infty$ this containment, in the case of ordinary shocks, occurs by deflection of the interface which in turn induces an oblique shock wave in the inert gas, and by transmission of an expansion wave or "expansion zone" into the region behind the incident shock[19] as shown in

Fig. 4. In the case of the detonation the shock wave is followed by a reaction zone within which the gases expand to sonic velocity and the pressure rapidly drops to the Chapman-Jouguet value at the sonic or C-J plane. If the detonation is viewed as a discontinuity then, when $a_5 < a_\infty$ the deflection and pressure conditions can be satisfied by transmission of an oblique shock into the inert gas and the propagation of a Prandtl-Meyer expansion into the region behind the detonation. This theoretical model, which has been verified experimentally by Sommers[1], however, provides no information about the interface flow within the reaction zone itself, which must be understood in order to calculate the interface angle α_i.

It is postulated that the flow at the edge of the interaction zone is as shown in Fig. 6. Along the interface, the pressure and flow direction in the reaction zone and in the supersonic region behind the induced shock must match. Some experimental support for this model is provided by the schlieren photograph of a quenching detonation moving past an inert gas as shown in Fig. 5. Here the combustion zone lags considerably behind the shock with the result that the incident and induced shock waves are clearly visible in the region between the shock and the reaction zone. With respect to the inert gas the reaction zone acts as a slender body on which a tangency and pressure condition must be satisfied while the surface shape is left free. These requirements are sufficient to determine the interface angle α_i, though the detailed calculation will be quite difficult. Clearly if α_i is too small, for example the extreme $\alpha_i = 0$, the induced shock will be unable to contain the pressure in the reaction zone; on the other hand, with α_i too large the pressure behind the induced shock will be too large. Fortunately the flow in this interaction region is isolated from the downstream flow by the C-J or sonic plane and by the region of supersonic flow behind the induced shock wave. To be consistent with the first order theory plane wave reaction zone pressures should be used to compute the flow in the above interaction region. It follows that to first order α_i will be independent of channel width and velocity decrement but will only depend on the properties of the explosive and inert gases.

The formulation of the curved front theory is essentially complete. Once α_i is determined equation (47) provides a relation between the velocity decrement η, and the channel width and reaction zone thickness L, and ℓ_o. The reaction zone thickness ℓ_o, can be obtained from the C-J condition, (45), evaluated at $\alpha = 0$, that is from the equation

$$\frac{\eta}{K_1 \epsilon \Lambda} \left(\frac{\rho^{(0)}}{\rho_\infty} - 1 \right)_{\bar{y}=1} = \sum_{\alpha} \sigma_\alpha \left. \frac{\partial \lambda_\alpha^{(0)}}{\partial \bar{y}} \right|_{\bar{y}=1} \tag{45a}$$

Application of the above theory requires detailed knowledge of the chemical processes within the reaction zone as well as computation of α_i. Exact solution of these two auxiliary problems is difficult and beyond the scope of the present work; however, to provide a preliminary test of the theory approximate velocity decrement calculations for stoichiometric H_2 - O_2 detonations have been made and compared with experimental results as described below.

IV. APPROXIMATE CLACULATION OF THE VELOCITY DECREMENTS OF A STOICHIOMETRIC H_2 - O_2 DETONATION

The combustion process has been approximated by the single first order reversible reaction

$$A_1 \rightleftarrows A_2 \quad .$$

such that there is no change in molecular weight. A similar scheme has been used by others [17, 20]. Then it is readily shown that

$$\sum_{\alpha} \sigma_{\alpha} \frac{d\lambda_{\alpha}^{(0)}}{dy} = \frac{Q}{C_p T} \frac{d\kappa_2^{(0)}}{\partial y} \tag{48}$$

where Q is the heat of reaction. For this first order reaction the reaction rate in terms of the mass concentrations becomes[20]

$$\frac{d\kappa_2^{(0)}}{dy} = \frac{\kappa_{2e}^{(0)} - \kappa_2^{(0)}}{v^{(0)} \tau \kappa_{2e}^{(0)}} \exp -\left(\frac{E_A}{\mathcal{R} T^{(0)}}\right) \tag{49}$$

where τ is a characteristic time, κ_{2e} the equilibrium mass concentration, and E_A the activation energy. For purposes of computing ℓ_o only the rate near the end of the reaction zone is required. If it is assumed that

$$\frac{1}{\lambda} = \frac{1}{\tau v^{(0)} \kappa_{2e}^{(0)}} \exp -\left(\frac{E_A}{\mathcal{R} T^{(0)}}\right) = \text{constant}$$

integration of Eq. (49) yields

$$\kappa_2^{(0)} = \kappa_{2e}^{(0)} \left[1 - \exp -\left(\frac{y}{\lambda}\right)\right] \quad . \tag{50}$$

This result, in which λ plays the role of a relaxation distance, was also used by Fay[17]. Following Fay it has been assumed that $\kappa_{2e}^{(0)} \cong 1.0$, that $(Q/C_p T) \cong 1.0$, and that $\lambda = 0.6$ mm for stoichiometric H_2 - O_2 detonations at 1 atmosphere.

To compute Λ the reaction zone density has been assumed constant and equal to the average of the density behind the shock and at the C-J plane so that

$$\Lambda = \left[\frac{1}{2}\left(\frac{\rho_1^{(0)}}{\rho_\infty} + \frac{\rho_2^{(0)}}{\rho_\infty}\right) - 1\right] \quad . \tag{51}$$

The density ratios in (51) were obtained from normal shock tables and the equilibrium calculations of Moyle[21]. For stoichiometric H_2 - O_2 detonations, $\rho_1^{(0)}/\rho_\infty = 5.06$, $\rho_2^{(0)}/\rho_\infty = 1.78$.

In order to compute α_i it has been assumed that the interface is straight and at an angle $1/2\ (\beta_1 + \beta_2)$ where β_1 and β_2 are the deflection angles at the shock and at the C-J plane (Fig. 6). Requiring the pressure behind the induced oblique shock to equal the pressure at the C-J plane then resulted in a value $\alpha_i = 13.3^{\circ}$ in the stoichiometric H_2 - O_2 case. Essentially it is assumed that the pressure rapidly drops to the final C-J value. A plane detonation velocity and Mach number of 9,250 ft/sec and 5.20, taken from Moyle were used in the calculation of α_i.

Finally Fay's values for K_1 and ϵ and that is $K_1 = 0.53$, $\epsilon = 1$, were used.

With the above information it was possible to simultaneously solve Eqs. (45a), and (47) for η and ℓ_o. The computed values of η are compared to the measurements of Dabora in Fig. 7 and it can be seen that there is reasonable agreement between theory and experiment. Figure 7 also indicates the decrease in reaction zone thickness with decreasing channel width. The results of Fig. 7 provide encouraging support for the present theory.

V. DISCUSSION

The first order theory developed above provides a relationship between the explosive-inert interface conditions and the velocity decrement and detonation curvature. The theory is essentially a hydrodynamic one without detailed consideration of chemical effects. Analysis of the problem of detonation stability and quenching limits, which is not considered in this paper, can undoubtedly be coupled to the present theory.

Laminar flow within the reaction zone has been assumed, though it is well known[22] that the structure of many C-J detonations is turbulent and that the wave surfaces may be non-uniform or crinkled. If it is reasonable to use temporal averages within distances of the order of the reaction zone thickness the theory developed here may still be applicable.

The agreement between the approximate calculations and Dabora's experimental results is reassuring; however, further verification would be desirable. In particular more precise values of $\rho^{(0)}/\rho_\infty$ and the pressure variation, should be used in the computation of Λ and α_i. Calculated values of α_i and wave curvature should be compared with values taken from Schlieren photographs, and the comparison of theory and experiment should be extended to wider ranges of mixture ratio. It should be possible to use the present theory to obtain chemical-kinetic information from Schlieren photographs and velocity decrement data from gaseous detonations with side relief.

Only the case in which the speed of sound in the inert is less than in the explosive was considered in the treatment of the interface flow. The curved front theory above should remain valid even in the case of higher sound speed in the inert gas. The chief difficulty in this more complex case lies in the calculation of the detailed interface flow.

The nature of the C-J condition requires further study, especially the nature of the transition from the plane to the curved front case.

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VII. NOMENCLATURE

L	width of explosive
D	detonation velocity
ρ	density
x, y	distance along and normal to wave
u, v	x, y velocity components
K	local wave curvature
R	wave radius of curvature
α	wave angle
p	pressure
h	static enthalpy
h_o	total enthalpy
X_s	unit mass of species s
ν_s^{α}	stoichiometric coefficient of species s in reaction α
λ_{α}	progress variable of αth reaction
r_{α}	rate of αth reaction
κ_s	mass fraction of species s
c_o	frozen speed of sound
$\hat{v}$	specific volume
C_p^o	frozen constant pressure specific heat
β_o	frozen expansion coefficient
ℓ_o	a characteristic reaction zone length
δ	ℓ_o/R
$\bar{x}$	dimensionless coordinate defined by $d\bar{x} = dx/R$
$\bar{y}$	y/ℓ_o
η	dimensionless velocity decrement
ℓ	reaction zone thickness
a_{∞}, a_5	sonic velocity of unreacted explosive and undisturbed inert gas respectively

Subscripts

$( )_1$	immediately behind the shock
$( )_2$	at the C-J plane
$( )_i$	at the explosive-inert interface

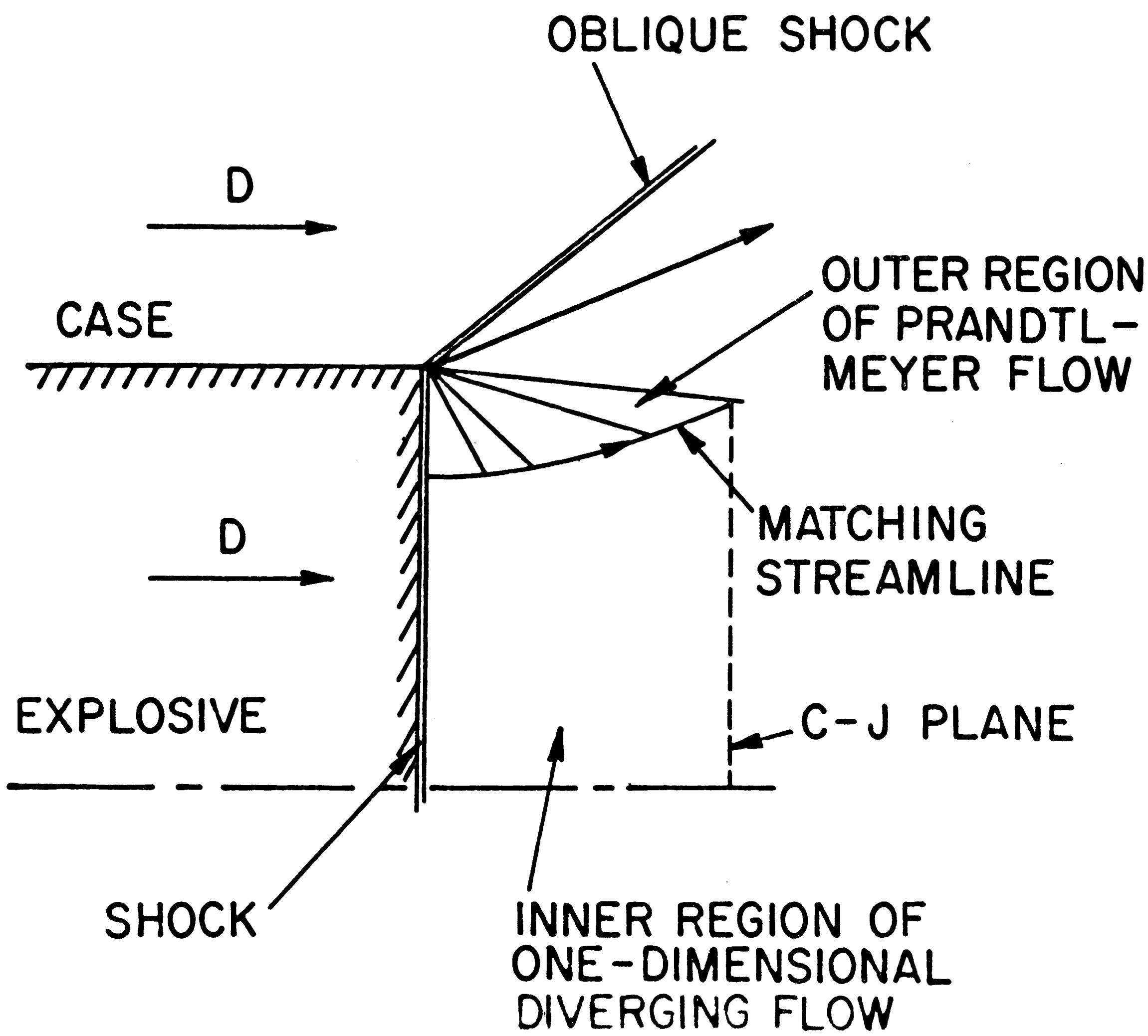


Fig. 1: Schematic Diagram of the Jones Model of a Detonation with Side Relief

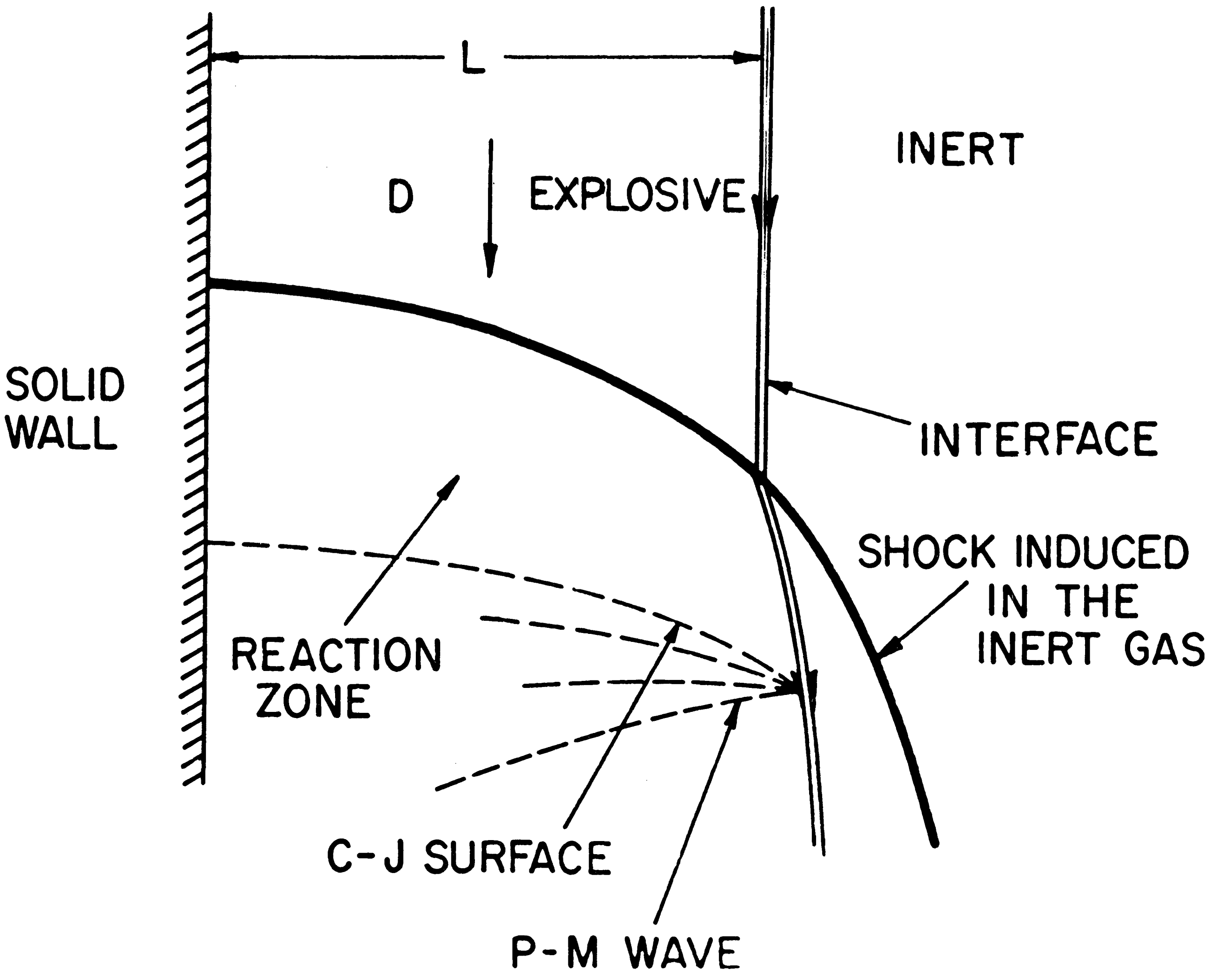
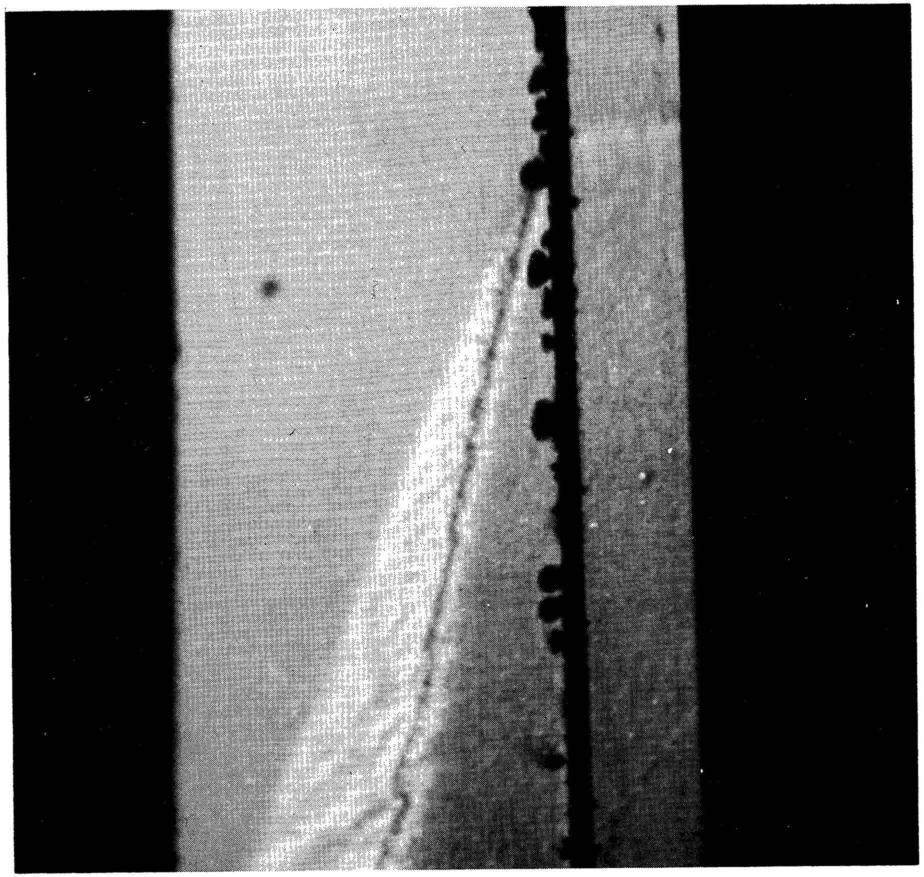


Fig. 2a: Schematic Diagram of a Two Dimensional Detonation Propagating through a Slab of Gaseous Explosive



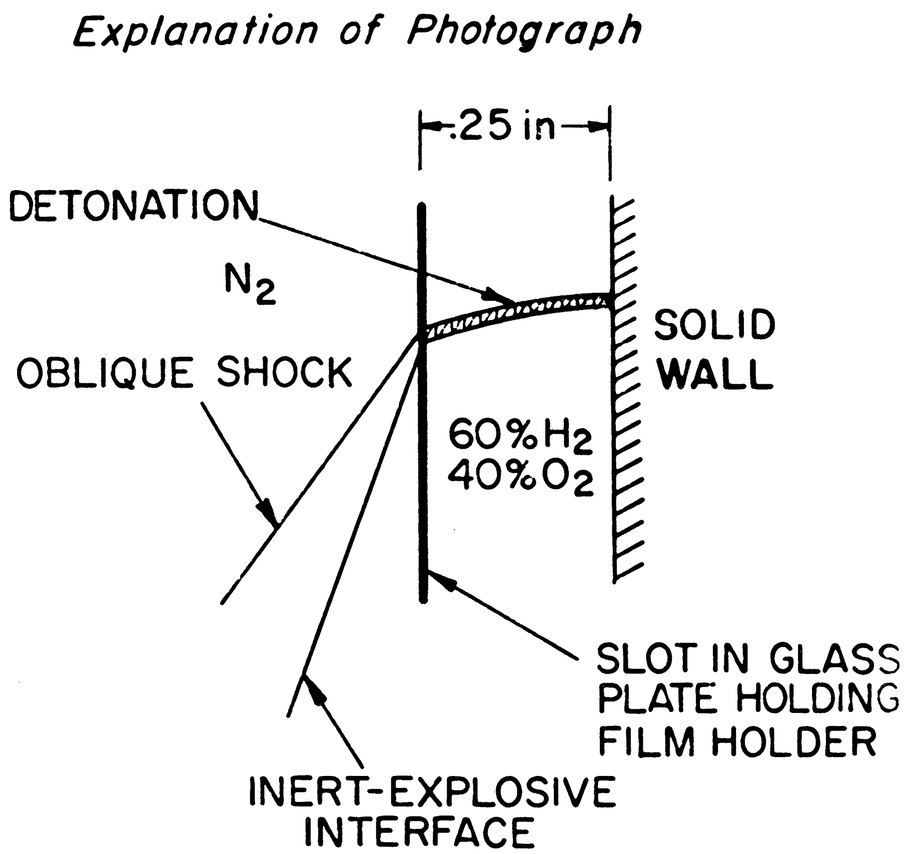
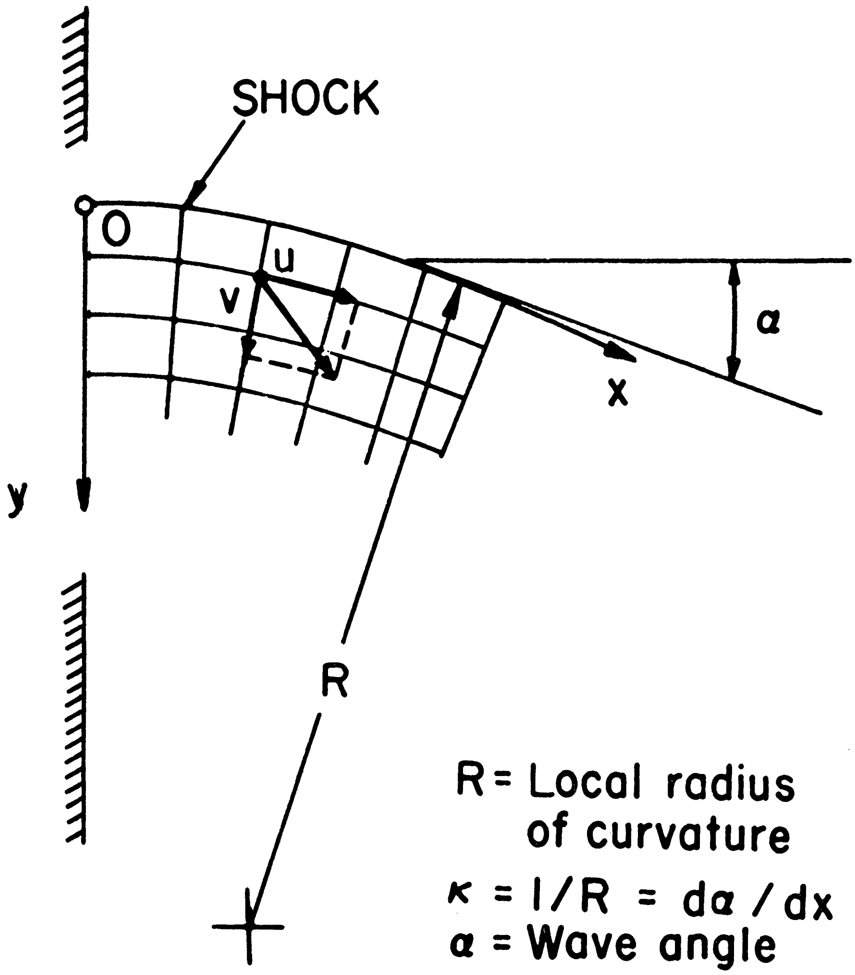


Fig. 2b: Schlieren Photo of Unquenched 60% H_2-40% O_2 Detonation Propagating in 0.25 in Channel Bounded by N_2 (Taken from Ref. 6). Explosive and Inert Separated by 250 Å Nitrocellulose Film.



$$ds^2 = (1 - \kappa y)^2 \, dx^2 + dy^2 \qquad \text{(Metric)}$$

Fig. 3. Shock Based Coordinates

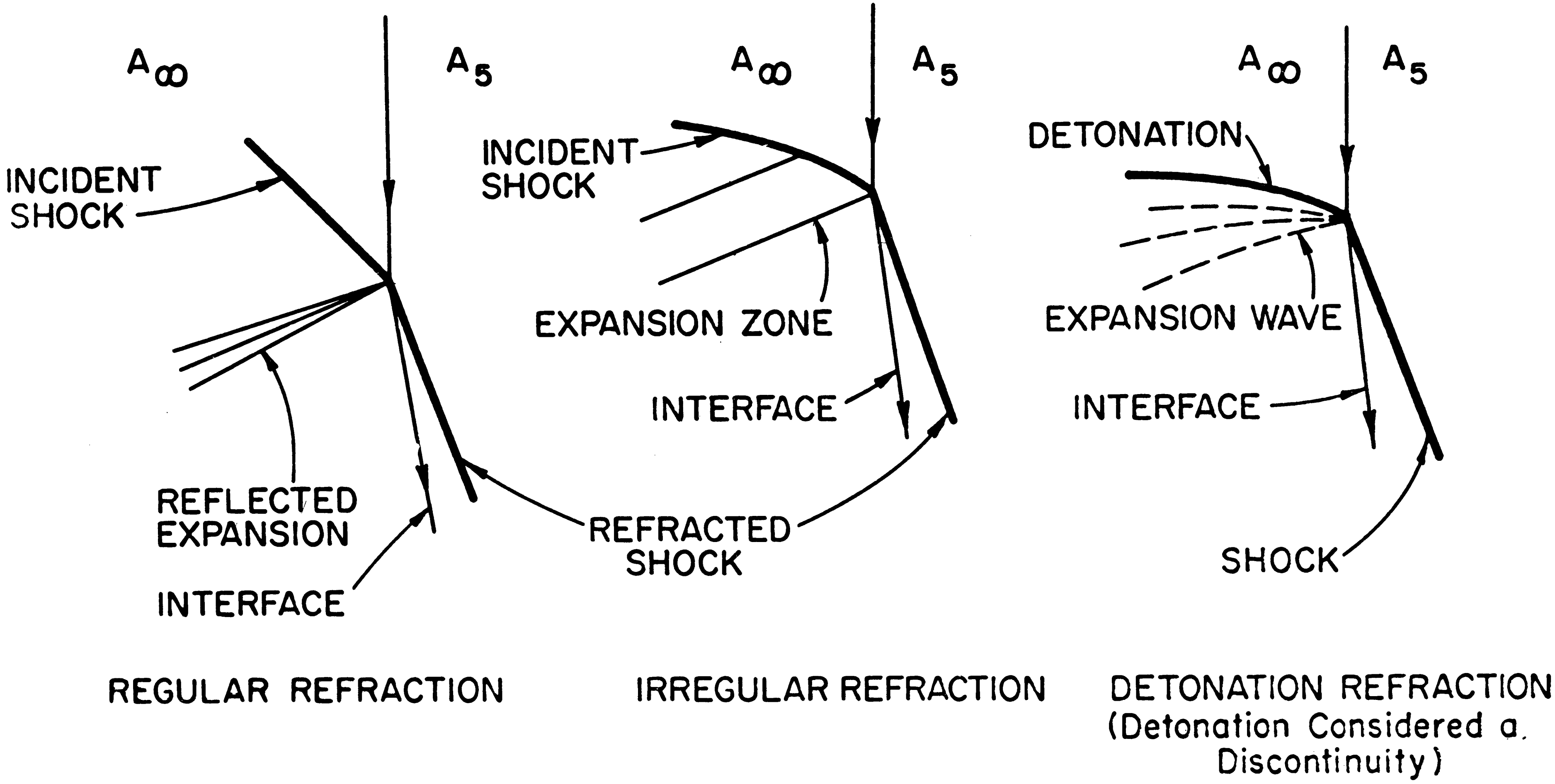
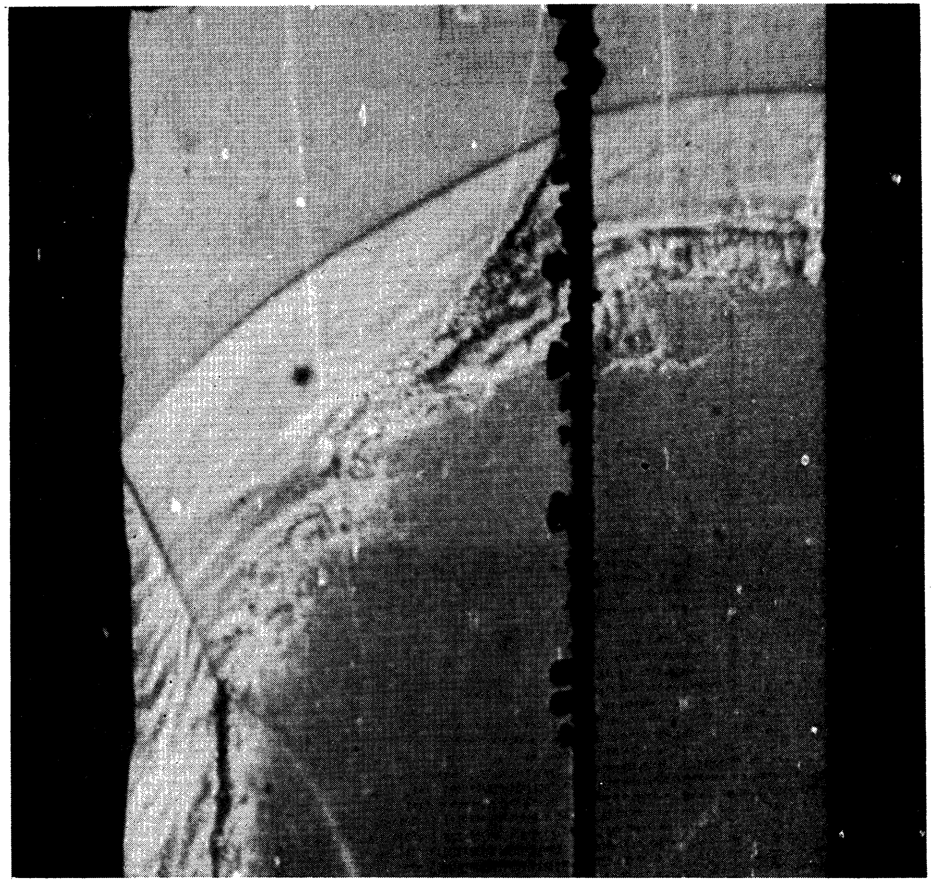


Fig. 4: Shock and Detonative Refractions $A_5 < A_\infty$



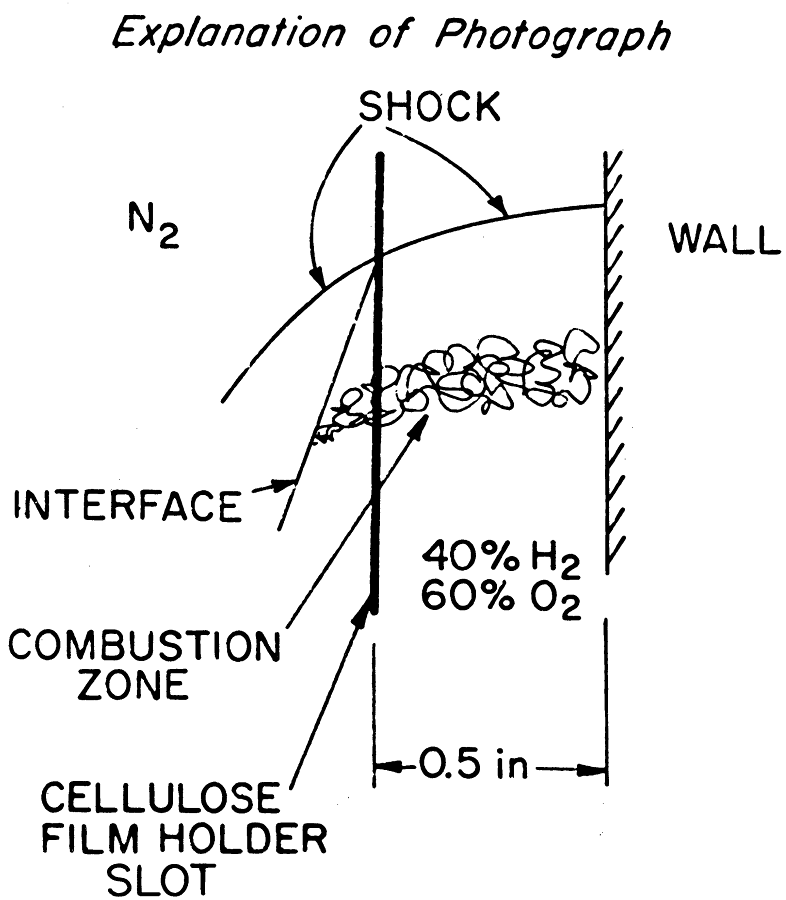


Fig. 5: Schlieren Photo of Quenching 40% H_2 - 60% O_2 Detonation (Taken from Ref. 6).

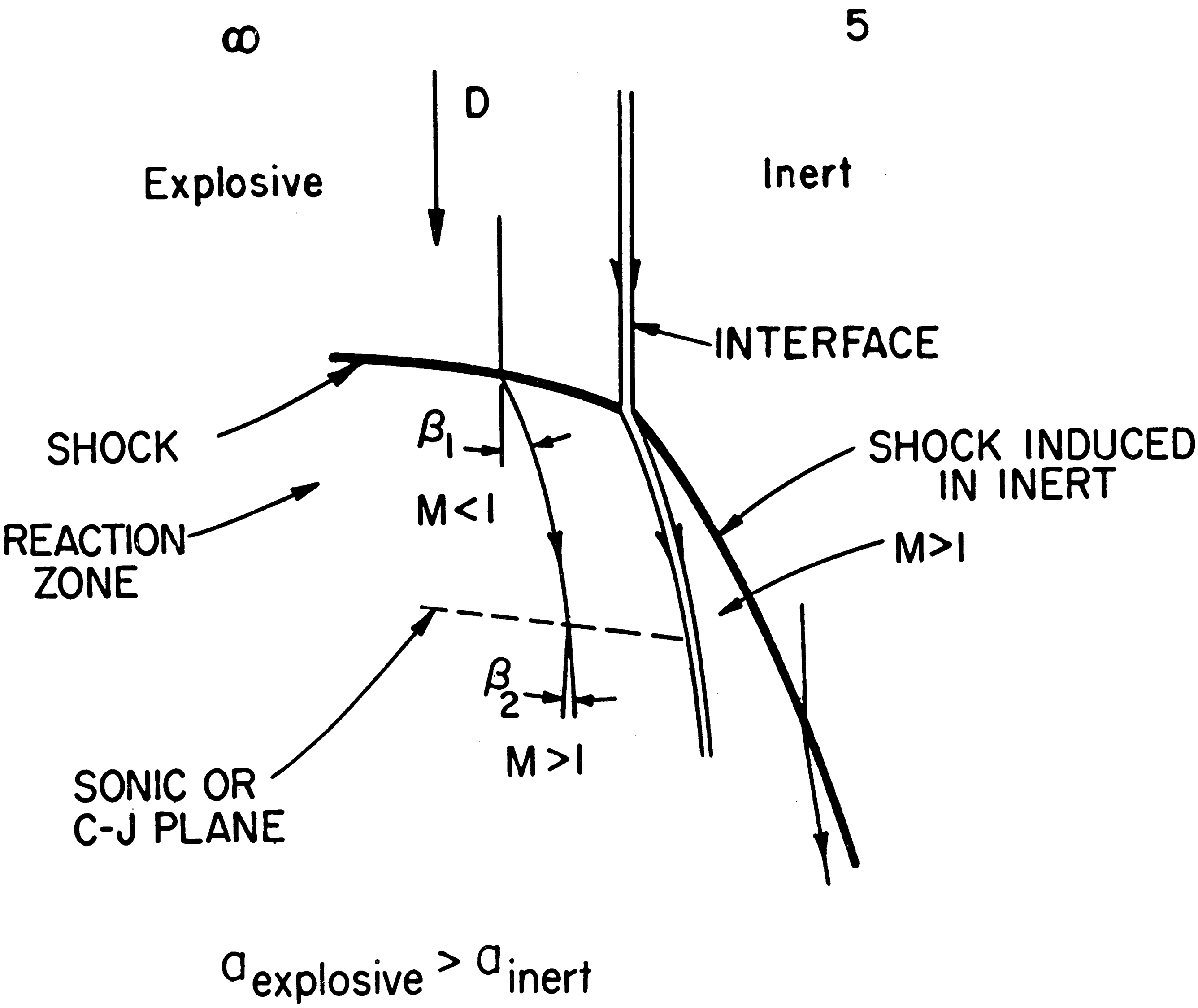


Fig. 6: Postulated Flow at the Edge of the Interaction Zone.

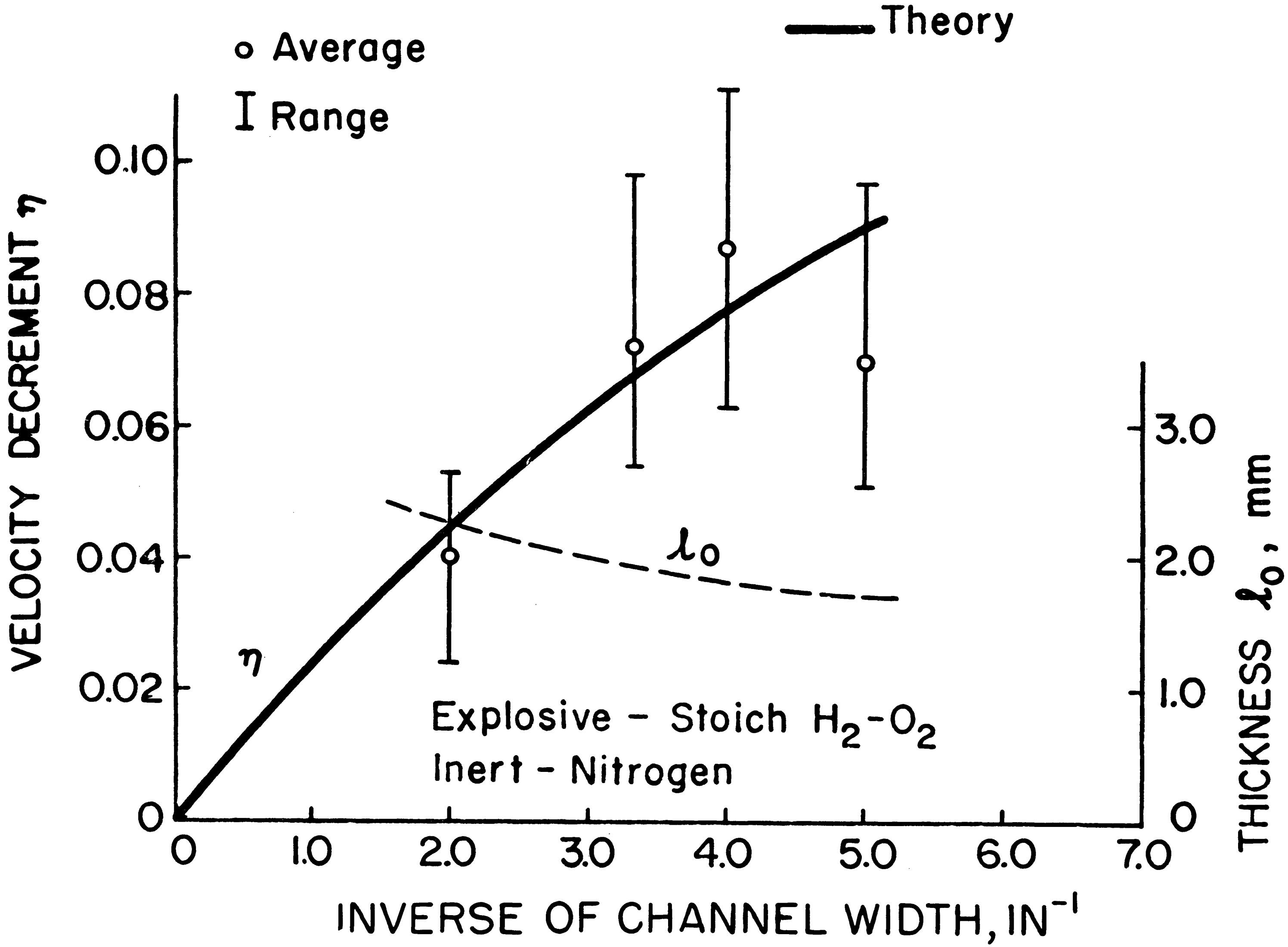


Fig. 7: Comparison of Theoretical Velocity Decrements with Measurements of Dabora (Ref. 6). Data Corrected for Wall Boundary Layer Effect.