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Equilibrium Structure
Of Thin Diffusion Flame Zone

By

PAUL M. CHUNG *and* VICTOR D. BLANKENSHIP

DECEMBER 1965

Prepared for

BALLISTIC SYSTEMS DIVISION
AIR FORCE SYSTEMS COMMAND
Norton Air Force Base, California

SAN BERNARDINO OPERATIONS
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FOREWORD

This report by Aerospace Corporation, San Bernardino Operations has been done under Contract No. AF 04(695)-669 as TR-669(S6240-10)-1. The Air Force program monitor is Major M. Mauldin, Jr., USAF (BSYDM). The dates of research for this report include the period February 1965 through August 1965. This report was submitted by the author in December 1965.

This technical report has been reviewed and is approved.

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UNCLASSIFIED ABSTRACT

EQUILIBRIUM STRUCTURE OF THIN DIFFUSION FLAME ZONE, by P. M. Chung and V. D. Blankenship	TR-669(S6240-10)-1 December 1965

The method of inner-and-outer expansions was used to analyze the initial broadening of a diffusion flame sheet caused by the nonvanishing equilibrium constant. Analytic expressions are derived for the thickness of the flame zone, and the position and the value of the maximum flame temperature. The thickness of the flame zone created by the nonvanishing equilibrium constant is found to be less than that created by the decreasing Damkohler number studied previously. Varying the stoichiometric coefficient of the fuel is found to affect the oxidant side of the flow to a greater degree than the fuel side itself, and vice versa. The problem of nonvanishing equilibrium constant is important when a fuel is injected into a hypersonic stream and the high energy of the stream begins to prevent the full release of the heat of combustion. (Unclassified Report)

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FIGURES

I. INTRODUCTION

In the combustion of initially unmixed reactants, when it is considered that the chemical kinetics is represented by the simple relationship

$$a\ (\text{oxidant}) + b\ (\text{fuel}) \underset{k_b}{\overset{k_f}{\rightleftharpoons}} d\ (\text{product}), \tag{1}$$

it is well known[1] that a diffusion flame sheet is established as

$$\Gamma_f = \text{Damkohler number} = \frac{\text{characteristic residence time}}{\text{characteristic reaction time}} \rightarrow \infty, \tag{2}$$

and at the same time

$$\frac{k_b}{k_f} = \text{equilibrium constant} \rightarrow 0.$$

For this limiting case, the combustion is completely controlled by the diffusion and heat transfer characteristics of the flow field alone. This independence of the combustion on the chemical reaction kinetics, together with the fact that the equilibrium constant is zero, enables one to postulate a certain set of conditions at the flame sheet, and to solve the governing equations rather simply[1,2].

When either the Damkohler number or the equilibrium constant is finite and nonvanishing, a zone of finite thickness instead of the thin sheet is required for combustion. Solution of the governing equations is then no longer simple, and usually only a full numerical treatment can satisfactorily describe the burning process. Such numerical analyses and certain empirical simplifications derived from the numerical results were given by Chung, et al[3] and Libby and Economos[4].

The most efficient combustion from the standpoint of heat release takes place as $\Gamma_f \to \infty$ and $k_b/k_f \to 0$ and, hence, as the thin flame sheet is established. It is, therefore, very helpful if one can quickly predict, without having to solve numerically, the values of the Damkohler number and equilibrium constant at which the flame sheet first begins to broaden and the flame temperature begins to drop. Also, one would gain a considerable insight into the development of diffusion flames by studying in detail the manner in which the flame sheet first broadens, and by studying the structure of the thin flame zone thus created. The above information, which is often difficult to obtain through a pure numerical analysis, can be deduced by a suitable perturbation analysis.

Mathematically, the flame sheet represents a singular point[1] since the second derivatives of temperature and reactant concentrations increase without limit as one approaches the sheet. (See Figure 1.) Therefore, the flame sheet broadening cannot be analyzed by the regular perturbation method. In order to perturb about the singular point, the technique of inner-and-outer expansions was successfully employed by Chung, et al[3] when the broadening was caused by the decreasing Damkohler number for the general combustion process given in Eq. (1). A similar method was shown[1] to be applicable when the flame sheet broadening was caused by the nonvanishing equilibrium constant, with $\Gamma_f \to \infty$, but only for $a = b = d = 1$. Unlike the flame zone[3] created by the decreasing Γ_f, relaxing the restriction of $a = b = d = 1$ to arbitrary stoichiometric coefficients does not result in a simple extension of the analysis for $a = b = d = 1$ if the broadening is caused by a nonvanishing equilibrium constant. It is because the flame sheet broadening by the decreasing Γ_f directly influences the inner region only whereas that due to the nonvanishing equilibrium constant directly affects both inner and outer regions and, hence, influences the matching process.

In the present paper, the initial broadening of the flame sheet caused by the nonvanishing equilibrium constant, for equilibrium flows, will be analyzed by the method of inner-and-outer expansions for arbitrary stoichiometric coefficients. From the analysis, closed form expressions will be derived for the important variables such as the value and the location of the maximum temperature of the flame zone.

II. FORMULATION

The basic chemical features of the present analysis are independent of any particular flow geometry. We shall hence consider the simple stagnation mixing layer configuration previously employed[3] for convenience. A jet of pure gaseous fuel is introduced into the oncoming uniform stream of pure oxidant at the stagnation region of a two dimensional or axisymmetric blunt body. A laminar mixing layer is then formed as the two streams meet (see Figure 2).

The general governing equations for this problem have been derived and appropriately transformed for Prandtl and Schmidt numbers of unity in the previous paper[3], from which we write when $\frac{1}{\Gamma_f} = 0$,

$$f''' + f f'' = 0 \tag{3}$$

$$(H + m_1)'' + f (H + m_1)' = 0 \tag{4}$$

$$(H + m_2)'' + f (H + m_2)' = 0 \tag{5}$$

$$m_1^a m_2^b - \epsilon H^{a+b} \exp\left(-\frac{\theta}{H}\right)\left(1 - \frac{a M_1}{M_3} m_1 - \frac{b M_2}{M_3} m_2\right) = 0 \tag{6}$$

where ϵ is the suitably normalized constant portion of the equilibrium constant and it is defined as

$$\epsilon = \frac{1}{a^a b^b} M_3^{a+b-1} \left(\frac{\Delta h^o}{c_p}\right)^{a+b} \left(\frac{P}{R}\right)^{1-(a+b)} K_{E0} \tag{7}$$

with the equilibrium constant expressed as

$$\frac{k_b}{k_f} = K_{E0} \, T^n \exp\left(-\frac{\Delta E}{RT}\right) . \tag{8}$$

The stoichiometric coefficient d is set to one in Eq. (1) without loss of generality because Eq. (1) can be always divided through by d, then a and b can be redefined. In Eq. (8), K_{E0} is a constant. The exponent n is set to one for Eq. (6)†. ΔE, R, P, and T are the heat of reaction per unit mass, gas constant per unit mass, pressure, and the temperature respectively. $\theta = (\Delta E\, c_p)/(R \Delta h^o)$ in Eq. (6) with the modified heat of reaction Δh^o defined as,

$$\Delta h^o = \frac{a M_1}{M_3} h_1^o + \frac{b M_2}{M_3} h_2^o - h_3^o \tag{9}$$

where h^o is the heat of formation per unit mass. c_p is the constant pressure specific heat of the gas mixture which is assumed to be constant. In Eqs. (3) through (5), $f(\eta)$ is the conventional Blasius stream function which is defined such that $f' = \frac{u}{u_e}$ where $(\ \ )'$ denotes the total differentiation with respect to the similarity variable η defined as

$$\eta = \left[\frac{(1+\sigma)}{\left(\rho_e \mu_e\right)_o} \left(\frac{du_e}{dx}\right)_o\right]^{1/2} \int_o^y \rho \, dy \quad . \tag{10}$$

---

† n = 0 was employed in Ref. 3.

In the above equation, σ is either zero or one depending on whether the flow is two dimensional or axisymmetric. u is the x-component of velocity as shown in Figure 2. The subscripts e and -e, denote the edges of the mixing layer on oxidant and fuel sides respectively, and o denotes the stagnation point. ρ and μ are the density and viscosity of the gas mixture respectively.

The subscripts 1, 2, and 3 represent the oxidant, fuel, and the combustion product respectively. H and m are the normalized temperature and mass fraction respectively defined as

$$H = \left(\frac{c_p}{\Delta h^o}\right) T,$$

$$m_1 = \left(\frac{M_3}{a\,M_1}\right) \hat{C}_1$$

$$m_2 = \left(\frac{M_3}{b\,M_2}\right) \hat{C}_2 \qquad (11)$$

where M and $\hat{C}$ represent the molecular weight and the mass fraction respectively.

The boundary conditions for the governing equations, Eqs. (3) through (6), are as follows:

For $\eta \to \infty$,

$$f' = 1,$$

$$H = H_e = \frac{c_p}{\Delta h^o} T_e,$$

$$m_1 = \frac{M_3}{a\,M_1} = m_{1e},$$

$$m_2 = 0, \qquad (12)$$

for $\eta \rightarrow -\infty$,

$$f' = \frac{u_{-e}}{u_e} = \lambda ,$$

$$H = H_{-e} = H_e \lambda^2 ,$$

$$m_1 = 0 ,$$

$$m_2 = \frac{M_3}{b\,M_2} = m_{2,-e} , \qquad (13)\dagger$$

and for $\eta = 0$,

$$f(0) = 0 . \qquad (14)$$

Though the equilibrium equation, Eq. (6), is algebraic, it automatically satisfies all the boundary conditions because the fluid is always in chemical equilibrium at both e and -e due to the fact that only one reactant is present at the mixing layer edges.

Now, we have completed the formulation of the boundary value problem which is comprised of Eqs. (3) through (6) and boundary conditions (12) through (14). Solution of this boundary value problem constitutes the next section.

III. ANALYSIS

The boundary value problem comprised of Eqs. (3) through (6) and Eqs. (12) through (14) will be analyzed in this section. The solution of momentum equation, Eq. (3), is available elsewhere[5,6] for some values of λ. In the present analysis, Eq. (3) was first integrated for various values of λ.

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† The particular flow geometry demands that $H_{-e}/H_e = \lambda^2$. This point was explained in detail in a previous paper.[3]

When $\epsilon = 0$, the boundary value problem can be solved readily by replacing Eq. (6) by a set of postulations derived from physical reasoning at the flame sheet. Such flame sheet solutions which a priori admit certain singularities at the sheet are well known[1,2,3,4]. When $\epsilon > 0$, on the other hand, Eq. (6) is highly nonlinear though algebraic, and the problem is in general amenable only to numerical analyses. The present interest, however, as was explained in Section I, is with the onset of the flame sheet broadening and the structure of the thin flame zone, thus with the small values of ϵ. We, therefore, shall obtain a perturbation solution of the boundary value problem posed with ϵ as the perturbing parameter. As it has been pointed out previously, $\epsilon = 0$ is a singular point and, hence, the regular perturbation technique cannot be applied to the present problem. In the following, the method of inner-and-outer expansions will be employed and closed form expressions which describe the salient features of the flame sheet broadening will be derived. For a general method of inner-and-outer expansions, the readers are referred to Van Dyke[7].

Asymptotic Expansions

We first assign an inner region about the singular point (the flame sheet) and represent it by (i). The remaining portion of the flow field is then designated as the outer region. We specify the outer region on the oxidant side as the upper outer region (u) and the fuel side the lower outer region (L). The superscript ( )* will be used to specify various values at the flame sheet which exists in the limit of $\epsilon = 0$. (See Figure 1.)

For the two outer regions, we express the dependent variables by the following regular series,

$$m_{1,u}(\epsilon, \eta) = Y_{u0}(\eta) + \epsilon^{j} Y_{u1}(\eta) + \epsilon^{2j} Y_{u2}(\eta) + O(\epsilon^{3j}),$$

$$m_{2,u}(\epsilon, \eta) = F_{u0}(\eta) + \epsilon^{j} F_{u1}(\eta) + \epsilon^{2j} F_{u2}(\eta) + O(\epsilon^{3j}),$$

$$H_{u}(\epsilon, \eta) = H_{u0}(\eta) + \epsilon^{j} H_{u1}(\eta) + \epsilon^{2j} H_{u2}(\eta) + O(\epsilon^{3j}), \qquad (15)$$

and

$$m_{1,L}(\epsilon,\eta) = Y_{L0}(\eta) + \epsilon^{k} Y_{L1}(\eta) + \epsilon^{2k} Y_{L2}(\eta) + O(\epsilon^{3k}),$$

$$m_{2,L}(\epsilon,\eta) = F_{L0}(\eta) + \epsilon^{k} F_{L1}(\eta) + \epsilon^{2k} F_{L2}(\eta) + O(\epsilon^{3k}),$$

$$H_{L}(\epsilon,\eta) = H_{L0}(\eta) + \epsilon^{k} H_{L1}(\eta) + \epsilon^{2k} H_{L2}(\eta) + O(\epsilon^{3k}). \qquad (16)$$

For the inner region, we first define a new independent variable with a stretching factor as

$$\zeta = \frac{\eta - \eta^*}{\epsilon^q} = \frac{\xi}{\epsilon^q} \qquad (17)$$

The dependent variables are then expressed by the series,

$$m_{1,i}(\epsilon,\zeta) = \epsilon^{\ell} \hat{Y}_1(\zeta) + \epsilon^{2\ell} \hat{Y}_2(\zeta) + O(\epsilon^{3\ell}),$$

$$m_{2,i}(\epsilon,\zeta) = \epsilon^{\ell} \hat{F}_1(\zeta) + \epsilon^{2\ell} \hat{F}_2(\zeta) + O(\epsilon^{3\ell}),$$

$$H_i(\epsilon,\zeta) = H^* + \epsilon^{\ell} \hat{H}_1(\zeta) + \epsilon^{2\ell} \hat{H}_2(\zeta) + O(\epsilon^{3\ell}). \qquad (18)$$

Now, it is crucial, in order for the inner-and-outer expansion method to work with the proposed series (15) through (18), that a particular set of constants j, k, q, and ℓ be found such that the ensuing solutions of the three regions will match in a consistent manner. The perturbation parameter appears explicitly only in Eq. (6) among the governing equations. Since ϵ appears in Eq. (6) as a linear parameter, one's natural tendency would be to expand the dependent variables for the outer regions, which are regular regions, into integral powers of ϵ. Indeed such expansions produced correct asymptotic solutions for the outer regions, which could be matched to the inner solution consistently to all order, when the flame sheet broadening was caused by the decreasing Damkohler number[3] for all values of a and b. Also, it was the case with the flame sheet broadening caused by a nonvanishing equilibrium constant[1] when $a = b = 1$. A similar attempt, however, was found to fail in the present analysis with arbitrary a and b. The physical reason why j and k should not necessarily be an integer will be discussed later. A careful study of the series, in the light of the governing equations, and the nature of the matching required, showed that the present method of solution would work only if we let

$$\begin{aligned} j &= 1/b, \\ k &= 1/a. \end{aligned} \tag{19}$$

For the inner region, in consideration of the fact that this region becomes finite as the second term of Eq. (6) which represents the backward reaction becomes non-negligible, and also the subsequent matching in mind, we let

$$q = \ell = 1/(a + b). \tag{20}$$

The above values of j, k, ℓ, and q will be shown to be correct later through matching. The series developed will now be used to analyze the various regions in the following subsections.

Outer Regions

The series (15) and (16), with the values given in Eqs. (19), are first substituted into the governing equations, Eqs. (4), (5), and (6), and a set of various order perturbation equations are generated for the outer regions by collecting the terms with equal powers of ϵ. The perturbation equations of Eqs. (4) and (5) are readily integrated in terms of the Blasius function f, and the boundary conditions specified by Eqs. (12) and (13) are applied to the zeroth order solutions for the upper and lower regions respectively. The usual homogeneous boundary conditions are satisfied by the higher order solutions. By applying the boundary conditions at $\eta \to \infty$ to the upper solutions and those at $\eta \to -\infty$ to the lower solutions, one of the two constants of integration of each order perturbation solution of Eqs. (4) and (5) is eliminated. The first two order solutions of Eqs. (4) and (5) and the corresponding perturbed equations of Eq. (6) thus derived for the outer regions are as follows:

$$\left\{\begin{aligned} &H_{u0} + Y_{u0} = A\,(f' - 1) + H_e + \frac{M_3}{a\,M_1}, && (21)\\ &H_{u0} + F_{u0} = C\,(f' - 1) + H_e, && (22)\\ &(Y_{u0})^a\,(F_{u0})^b = 0, && (23)\end{aligned}\right.$$

$$\left\{\begin{aligned} &H_{u1} + Y_{u1} = A_2\,(f' - 1), && (24)\\ &H_{u1} + F_{u1} = C_2\,(f' - 1), && (25)\\ &(Y_{u0})^a\,(F_{u1})^b = (H_{u0})^{a+b}\left(1 - \frac{a\,M_1}{M_3}\,Y_{u0}\right)\exp\left(-\frac{\theta}{H_{u0}}\right), && (26)\end{aligned}\right.$$

$$\left\{\begin{aligned} &H_{L0} + Y_{L0} = B\,(f' - \lambda) + H_{-e}, && (27)\\ &H_{L0} + F_{L0} = D\,(f' - \lambda) + H_{-e} + \frac{M_3}{b\,M_2}, && (28)\\ &(Y_{L0})^a\,(F_{L0})^b = 0, && (29)\end{aligned}\right.$$

$$\left\{\begin{aligned} &H_{L1} + Y_{L1} = B_2\,(f' - \lambda), && (30)\\ &H_{L1} + F_{L1} = D_2\,(f' - \lambda), && (31)\\ &(Y_{L1})^a\,(F_{L0})^b = (H_{L0})^{a+b}\left(1 - \frac{b\,M_2}{M_3}\,F_{L0}\right)\exp\left(-\frac{\theta}{H_{L0}}\right). && (32)\end{aligned}\right.$$

In the above equations, A, C, A_2, B, D, B_2, and D_2 are the remaining constants of integration which will be determined subsequently through matching.

As mentioned earlier, a flame sheet is established when $\epsilon = 0$. The well known flame sheet solution is obtained for the present problem by applying certain boundary conditions at η^* to Eqs. (21), (22), (27), and (28), and by thus determining the constants, A, C, B, and D. The flame sheet solution was given in the previous paper[3] from which we write for the subsequent use,

$$H^*_{u0} = H^*_{L0} = H^* = \frac{m_{1e}\, m_{2,-e} + H_{-e}\, m_{1e} + H_e\, m_{2,-e}}{m_{1e} + m_{2,-e}} \tag{33}$$

$$Y^*_{u0} = Y^*_{L0} = F^*_{u0} = F^*_{L0} = 0, \tag{34}$$

$$f'(\eta^*) = \lambda + \frac{m_{2,-e}(1 - \lambda)}{m_{1e} + m_{2,-e}} \tag{35}$$

Inner Region

A substitution of the series, Eqs. (18), with the aid of Eq. (20), into the governing equations, Eqs. (4), (5), and (6), and the collection of the terms with like powers of ϵ results in a set of perturbation equations for the inner region. The perturbation equations generated from Eqs. (4) and (5) are integrated readily. The first order inner solutions are given by,

$$\hat{H}_1 + \hat{Y}_1 = \alpha \zeta + \beta, \tag{36}$$

$$\hat{H}_1 + \hat{F}_1 = \gamma \zeta + \delta, \tag{37}$$

$$(\hat{Y}_1)^a (\hat{F}_1)^b = (H^*)^{a+b} \exp\left(- \frac{\theta}{H^*}\right), \tag{38}$$

where α, β, γ, and δ are the constants of integration.

With the use of the lowest order expressions derived for the outer and inner regions, the dependent variables will now be matched between the regions.

Matching

In view of the governing equations, Eqs. (4), (5), and (6), we shall match the functions $(H + m_1)$ $(H + m_2)$, and $(m_1)^a$ $(m_2)^b$, between the two outer regions and the inner region, to the lowest order. First, by matching the functions $(H + m_1)$ and $(H + m_2)$, all the unknown constants to the lowest order, A, C, B, D, α, β, γ, and δ will be determined. With the constants determined, it will be shown that the functions $(m_1)^a$ $(m_2)^b$ also match consistently thus completing the solution.

The function $(H + m_1)$ is first matched between the upper outer region and the inner region in the following manner. We obtain for the upper outer region with the aid of Eqs. (15),

$$H_u + m_{1u} = (H_{u0} + Y_{u0}) + \epsilon^{\frac{1}{b}} (H_{u1} + Y_{u1}) + O\left(\epsilon^{\frac{2}{b}}\right). \tag{39}$$

Eq. (39) becomes as $\eta \rightarrow \eta^*$, with the aid of Eqs. (33) and (34)

$$H_u + m_{1u} = H^* + \xi (H'_{u0} + Y'_{u0})^* + \frac{\xi^2}{2} (H''_{u0} + Y''_{u0})^* + O(\xi^3) + O\left(\epsilon^{\frac{1}{b}}\right). \tag{40}$$

In terms of the inner variable, Eq. (40) becomes with the aid of Eqs. (17) and (21),

$$H_u + m_{1u} = A(f'^* - 1) + H_e + \frac{M_3}{a M_1} + \epsilon^{\frac{1}{a+b}} \zeta A f''^* + O(\epsilon^{\frac{1}{b}}) + O\left(\epsilon^{\frac{2}{a+b}}\right). \tag{41}$$

Here either $\epsilon^{\frac{1}{b}}$ or $\epsilon^{\frac{2}{a+b}}$ may be greater than the other.

The function $(H + m_1)$ for the inner region becomes, with the aid of Eqs. (18) and (36),

$$H_i + m_i = H^* + \epsilon^{\frac{1}{a+b}} (\alpha \zeta + \beta) + O\left(\epsilon^{\frac{2}{a+b}}\right). \tag{42}$$

Eq. (42) becomes in the outer variable as

$$H_i + m_i = H^* + \alpha\,\xi + \epsilon^{\frac{1}{a+b}}\,\beta + O\left(\epsilon^{\frac{2}{a+b}}\right). \qquad (43)$$

A comparison of Eqs. (41) and (43) shows that a consistent matching up to $O\left(\epsilon^{\frac{1}{b}}\right)$ or $O\left(\epsilon^{\frac{2}{a+b}}\right)$, whichever is greater, will be accomplished for function $(H + m_1)$ if all the explicit terms of Eq. (41) can be matched with those of Eq. (43). Eq. (42) is equivalent to Eq. (43) except that the former is in the inner variable. We therefore match the explicit term of Eq. (42) with those of Eq. (41), and we obtain

$$A = \frac{H_e + \frac{M_3}{a\,M_1} - H^*}{1 - f'^*},$$

$$\alpha = A\,f''^*,$$

$$\beta = 0. \qquad (44)$$

In a similar manner, the function $(H + m_2)$ is matched between the upper outer and the inner regions. The functions $(H + m_1)$ and $(H + m_2)$ are also matched to the lowest order, in the same way, between the lower outer regions and the inner region. From these matchings the following results are obtained:

$$C = \frac{H_e - H^*}{1 - f'^*},$$

$$\gamma = \frac{(H_e - H^*)\,f''^*}{1 - f'^*},$$

$$\delta = 0,$$

$$B = A,$$

$$D = C. \qquad (45)$$

Now, all the constants of integration for Eqs. (21) through (23), (27) through (29), and (36) through (38) have been determined by matching functions $(H + m_1)$ and $(H + m_2)$. Notice, however, that the matching of these two functions could have been just as well accomplished with many other values of j, k, ℓ, and q, instead of those employed in the present problem. We shall now employ the crucial equation, Eq. (6), and match the function $(m_1)^a\ (m_2)^b$, and thereby show that only the particular values of j, k, ℓ, and q given by Eqs. (19) and (20) permit the function $(m_1)^a\ (m_2)^b$ to match consistently between the two outer regions and the inner region.

We derive for the upper outer region with the aid of Eqs. (6) and (15),

$$(m_{1u})^a\ (m_{2u})^b = \epsilon\ (H_{u0})^{a+b}\left(1 - \frac{a\,M_1}{M_3}\ Y_{u0}\right)\exp\left(-\frac{\theta}{H_{u0}}\right) + O\left(\epsilon^{1+\frac{1}{b}}\right). \tag{46}$$

The above equation becomes as $\eta \to \eta^*$, $(\xi \to 0)$,

$$\begin{aligned}(m_{1u})^a\ (m_{2u})^b = \epsilon\ \Bigg\{&(H_{u0}^{a+b})^*\left(1 - \frac{a\,M_1}{M_3}\ Y^*_{u0}\right)\exp\left(-\frac{\theta}{H^*_{u0}}\right)\\ &+ \xi\left[-(H_{u0}^{a+b})^*\ \frac{a\,M_1}{M_3}\ (Y'_{u0})^*\ \exp\left(-\frac{\theta}{H^*_{u0}}\right) + (H_{u0}^{a+b})^*\left(1 - \frac{a\,M_1}{M_3}\ Y^*_{u0}\right)\cdot\right.\\ &\frac{(H'_{u0})^*}{(H_{u0}^2)^*}\ \theta\cdot\exp\left(-\frac{\theta}{H^*_{u0}}\right) + (a+b)\left(H_{u0}^{a+b-1}\right)^*(H'_{uo})^*\left(1 - \frac{a\,M_1}{M_3}\ Y^*_{u0}\right)\cdot\\ &\left.\exp\left(-\frac{\theta}{H^*_{u0}}\right)\right] + O\,(\xi^2)\Bigg\} + O\left(\epsilon^{1+\frac{1}{b}}\right),\end{aligned} \tag{47}$$

which becomes with the aid of Eqs. (21) through (23), as $\eta \rightarrow \eta^*$ ($\xi \rightarrow 0$),

$$(m_{1u})^a (m_{2u})^b = \epsilon \left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right] + \epsilon \left\{ \xi \exp\left(-\frac{\theta}{H^*}\right) \cdot \left[-\frac{a M_1}{M_3} (A-C)(H^*)^{a+b} + C\theta (H^*)^{a+b-2} + C(a+b)(H^*)^{a+b-1} \right] f''^* + O(\xi^2) \right\} + O\left(\epsilon^{1+\frac{1}{b}}\right), \tag{48}$$

For the inner region, we derive with the aid of Eqs. (6) and (18),

$$(m_{1i})^a (m_{2i})^b = \epsilon (H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) + \epsilon^{1+\frac{1}{a+b}} \left[-\frac{a M_1}{M_3} \hat{Y}_1 (H^*)^{a+b} - b\frac{M_2}{M_3} \hat{F}_1 (H^*)^{a+b} + (a+b)(H^*)^{a+b-1} \hat{H}_1 + (H^*)^{a+b-2} \hat{H}_1 \theta \right] \cdot \exp\left(-\frac{\theta}{H^*}\right) + O\left(\epsilon^{1+\frac{2}{a+b}}\right). \tag{49}$$

Now, before we can analyze the behavior of the above equation as $\zeta \rightarrow \infty$, we must find the behavior of functions $\hat{Y}_1(\zeta)$, $\hat{F}_1(\zeta)$ and $\hat{H}_1(\zeta)$ for large values of ζ. These are obtained in the following.

The first order inner expressions, Eqs. (36), (37), and (38), are first manipulated to give

$$(\hat{F}_1)^{\frac{a+b}{a}} + (\alpha - \gamma)\zeta (\hat{F}_1)^{\frac{b}{a}} - \left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{a}} = 0. \tag{50}$$

Solution of above algebraic equation is not usually obtainable in closed form for arbitrary values of a and b. However, for the purpose at hand which is to derive analytic expressions for $\hat{Y}_1$, $\hat{F}_1$ and $\hat{H}_1$ for large positive values of ζ, an asymptotic solution of Eq. (50) is obtained as,

$$\hat{F}_1(\zeta) = \left\{ \frac{\left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{a}}}{(\alpha-\gamma)\zeta} \right\}^{\frac{a}{b}} - \left(\frac{a}{b}\right) \frac{1}{(\alpha-\gamma)\zeta} \left\{ \frac{\left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{a}}}{(\alpha-\gamma)\zeta} \right\}^{\frac{2a}{b}} + O\left(\frac{1}{\zeta^{2+\frac{3a}{b}}} \right). \qquad (51)$$

The asymptotic expressions for functions $\hat{Y}_1$ and $\hat{H}_1$ are similarly derived as

$$\hat{Y}_1(\zeta) = (\alpha-\gamma)\zeta + \left\{ \frac{\left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{a}}}{(\alpha-\gamma)\zeta} \right\}^{\frac{a}{b}} + O\left(\frac{1}{\zeta^{1+\frac{2a}{b}}} \right), \qquad (52)$$

$$\hat{H}_1(\zeta) = \gamma\zeta - \left\{ \frac{\left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{a}}}{(\alpha-\gamma)\zeta} \right\}^{\frac{a}{b}} + O\left(\frac{1}{\zeta^{1+\frac{2a}{b}}} \right). \qquad (53)$$

Now, having derived the expressions for functions $\hat{F}_1$, $\hat{Y}_1$, and $\hat{H}_1$ for large positive values of ζ, we return to Eq. (49).

With the aid of Eqs. (51), (52), and (53), Eq. (49) becomes as $\zeta \to \infty$,

$$
\begin{aligned}
(m_{1i})^a (m_{2i})^b = {} & \epsilon \, (H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) + \epsilon^{1+\frac{1}{a+b}} \exp\left(-\frac{\theta}{H^*}\right) \cdot \\
& \Bigg\{ \left[(a+b)\,(H^*)^{a+b-1}\,\gamma + (H^*)^{a+b-2}\,\theta\,\gamma - (H^*)^{a+b} \left(\frac{a\,M_1}{M_3}\right)(\alpha - \gamma) \right] \zeta \\
& - \left[(a+b)\,(H^*)^{a+b-1} + (H^*)^{a+b-2}\,\theta + (H^*)^{a+b}\,\frac{a\,M_1}{M_3} + (H^*)^{a+b}\,\frac{bM_2}{M_3} \right] \cdot \\
& \frac{\left[(H^*)^{a+b} \exp\left(-\frac{\theta}{H^*}\right) \right]^{\frac{1}{b}}}{(\alpha - \gamma)\,\zeta^{\frac{a}{b}}} \Bigg\} + O\left(\epsilon^{1+\frac{2}{a+b}}\right). \qquad (54)
\end{aligned}
$$

Above equation becomes in terms of the outer variable,

$$
\begin{aligned}
(m_{1i})^a (m_{2i})^b = {} & \epsilon \exp\left(-\frac{\theta}{H^*}\right) \Bigg\{ (H^*)^{a+b} + \Bigg[(a+b)\,(H^*)^{a+b-1}\,\gamma \\
& + (H^*)^{a+b-2}\,\theta\,\gamma - (H^*)^{a+b}\,(\alpha - \gamma)\,\frac{a\,M_1}{M_3} \Bigg] \xi \Bigg\} \\
& + O\left(\epsilon^{1+\frac{1}{b}}\right) + O\left(\epsilon^{1+\frac{2}{a+b}}\right). \qquad (55)
\end{aligned}
$$

Now, the outer solution as $\eta \to \eta^*$ will be matched to the inner solution as $\zeta \to \infty$. This can be done by matching Eq. (48) with Eq. (55). With the help of Eqs. (44) and (45), which define and relate various constants, it is readily seen that all the explicit terms of Eq. (48) match with those of Eq. (55). A similar matching can be established between $(m_{1L})^a\,(m_{2L})^b$ and $(m_{1i})^a\,(m_{2i})^b$.

Now, we have accomplished the complete first order matching between the two outer regions and the inner region.

With the present values of j, k, ℓ, and q, the higher order matchings can also be carried out but with increasing algebraic complexities. Also, it is noted here that any other values of j, k, ℓ, and q do not permit the matching of the function $(m_1)^a\,(m_2)^b$.

Maximum Flame Zone Temperature and the Location

From Eqs. (18),

$$H_i = H^* + \epsilon^{\frac{1}{a+b}}\,\hat{H}_1 + O\left(\epsilon^{\frac{2}{a+b}}\right), \tag{56}$$

and from Eq. (37),

$$\hat{H}_1 = \gamma\zeta - \hat{F}_1 \tag{57}$$

In order to obtain the first order inner functions, $\hat{H}_1(\zeta)$, $\hat{Y}_1(\zeta)$, and $\hat{F}_1(\zeta)$, for all values of ζ, the algebraic equations, Eqs. (36), (37), and (38), must be solved. This entails the general solution† of a nonlinear algebraic equation, Eq. (50). For most cases of combustion, however, the primary interest is with the value and the location of the maximum flame temperature as affected by the flame sheet broadening. These informations can be obtained without the general solution of Eq. (50). In the following, analytical expressions will be derived for the value and the location of the maximum temperature of the broadening flame zone.

The maximum value of H_i exists where

$$\left(\frac{dH_i}{d\zeta}\right)_m = \epsilon^{\frac{1}{a+b}}\left[\gamma - \left(\frac{d\hat{F}_1}{d\zeta}\right)_m\right] = 0 \tag{58}$$

to $O\left(\epsilon^{\frac{1}{a+b}}\right)$. Thus $(H_i)_m$ occurs where

$$\left(\frac{d\hat{F}_1}{d\zeta}\right)_m = \gamma \tag{59}$$

---

†Note that only the asymptotic solution of Eq. (50) for large values of ζ, obtained analytically, was needed for the matching.

First, we shall evaluate $(\hat{F}_1)_m$, where $(\ \ )_m$ denotes the value at the position of the maximum flame zone temperature. Note that $\eta_m = \eta^*$ when $\epsilon = 0$. We differentiate Eq. (50) with respect to ζ and substitute γ for $\frac{d\hat{F}_1}{d\zeta}$ in accordance with Eq. (59). The resulting equation is then readily solved for $(F_1)_m$ as

$$(\hat{F}_1)_m = - \left[\frac{(\alpha - \gamma)\, \gamma \left(\frac{b}{a}\right)}{\alpha + \gamma \left(\frac{b}{a}\right)} \right] \zeta_m \ . \tag{60}$$

Eq. (60) is now substituted back into Eq. (50) and the resulting equation is solved for ζ_m. Then, we obtain for the location of the maximum flame zone temperature,

$$\eta - \eta^* = \epsilon^{\frac{1}{a+b}} \left[\exp\left(- \frac{\theta}{H^*} \right) \right]^{\frac{1}{a+b}} \frac{H^* (1 - f'^*) \left[\frac{M_3}{aM_1} + \frac{M_3}{bM_2} - \left(\frac{a+b}{a}\right) \left(\frac{M_3}{bM_2} + H_{-e} - H_e \right) \right]}{\frac{M_3}{aM_1} f''^* \left[\left(\frac{b}{a}\right)^b \left(\frac{M_3}{bM_2} + H_{-e} - H_e \right)^b \left(\frac{M_3}{aM_1} + H_e - H_{-e} \right)^a \right]^{\frac{1}{a+b}}} \ . \tag{61}$$

or,

$$\eta - \eta^* = \epsilon^{\frac{1}{a+b}} \left[\exp\left(- \frac{\theta}{H^*} \right) \right]^{\frac{1}{a+b}} \cdot$$

$$\frac{\left[\frac{M_3}{aM_1 M_2} (M_2 - M_1) - \left(\frac{a+b}{a}\right) (H_{-e} - H_e) \right] H^* (1 - f'^*)}{\left(\frac{M_3}{aM_1} \right) f''^* \left[\left(\frac{b}{a}\right)^b \left(\frac{M_3}{bM_2} + H_{-e} - H_e \right)^b \left(\frac{M_3}{aM_1} + H_e - H_{-e} \right)^a \right]^{\frac{1}{a+b}}} \ . \tag{62}$$

to $O\left(\epsilon^{\frac{2}{a+b}} \right)$.

Eqs. (60) and (61) or (62) give

$$(\hat{F}_1)_m = \left[\frac{b\left(\frac{M_3}{bM_2} + H_{-e} - H_e\right)}{a\left(\frac{M_3}{aM_1} + H_e - H_{-e}\right)}\right]^{\frac{a}{a+b}} H^* \left[\exp\left(-\frac{\theta}{H^*}\right)\right]^{\frac{1}{a+b}} . \tag{63}$$

$(H_i)_m$ then follows from Eqs. (56), (57), (61), (62), and (63), with some manipulation, as

$$(H_i)_m = H^* - \epsilon^{\frac{1}{a+b}} \left[\exp\left(-\frac{\theta}{H^*}\right)\right]^{\frac{1}{a+b}} \left(\frac{aM_1}{M_3}\right)\left(\frac{a}{b}\right)^{\frac{b}{a+b}} \left(1 + \frac{b}{a}\right) \cdot$$

$$(H^*)\,(H^* - H_e)^{\frac{a}{a+b}} \left(H_e - H^* + \frac{M_3}{aM_1}\right)^{\frac{b}{a+b}} + O\left(\epsilon^{\frac{2}{a+b}}\right) . \tag{64}$$

The properties at the thin flame sheet, $(\quad)^*$, are given in Eqs. (33) through (35). Now having derived the analytic expressions which describe the behavior of the maximum flame temperature, the results will be discussed in the following section.

IV. DISCUSSION

First, it is seen from Eqs. (17) and (20) that the order of the thickness of the flame zone created by the nonvanishing equilibrium constant is $\epsilon^{\frac{1}{a+b}}$. In the previous work^3, the order of the flame zone thickness created by decreasing Damkohler number was $(\epsilon_D)^{\frac{1}{a+b+1}}$ where ϵ_D is the reciprocal of

Damkohler number. Thus, the thickness of the flame zone created by a finite equilibrium constant is less than that created by a decreasing Damkohler number when a and b are order 1.

It was found[3] that all the perturbation terms in the outer regions except the zeroth order terms were found to be zero in the analysis of flame sheet broadening due to a decreasing Damkohler number. Hence, there[3] the outer regions were unaffected by the broadening flame sheet to all orders. This is the reason the expansions of the outer functions were not influenced by the stoichiometric coefficients, and were in integral powers of ϵ_D for all values of a and b. In the present problem, on the other hand, it was seen in Section III that the expansions of the outer functions depended directly on a and b. Also, it was seen, in that section, that the higher order outer terms were not zero but would have matched consistently to the appropriate inner terms. Thus, the effect of broadening flame sheet is felt in the outer regions, as well as in the inner region, when the broadening is caused by a nonvanishing equilibrium constant. We also see from Eqs. (15), (16), and (19) that increasing the stoichiometric coefficient of the fuel supplied from the lower outer region enhances the effect of the present flame sheet broadening on the upper outer region, rather than the lower region. Similarly, the stoichiometric coefficient of oxidant supplied from the upper region affects the lower region more than the upper region itself. Eq. (62) shows the location of the maximum flame temperature of a broadened zone with respect to that of the flame sheet. We see that the sign of the quantity $\left[\frac{M_3}{aM_1M_2}(M_2 - M_1) - \left(\frac{a+b}{a}\right)\left(H_{-e} - H_e\right)\right]$ determines the direction to which the position of the maximum temperature begins to move at the onset of the flame sheet broadening. It is seen that when $M_2 = M_1$ and $H_{-e} = H_e$ the position of the maximum temperature is unchanged and is at η^*. It is interesting to note that the position of the maximum flame temperature tends to move toward the lighter reactant (reactant with a smaller molecular weight) as the flame sheet is broadened. Also, it would move toward higher temperature reactant source. Moreover, increasing the stoichiometric coefficients a and b will accentuate the temperature effect, as compared to the molecular weight effect, on the movement of the position of the maximum temperature. One can readily manipulate the results given in the previous paper[3] and show, when the flame zone is created by the decreasing Damkohler number, that the position of the maximum flame temperature is governed by the parameter,

$$\frac{b\ M_2\ (H^* - H_{-e}) - a\ M_1\ (H^* - H_e)}{b\ M_2\ (H^* - H_{-e}) + a\ M_1\ (H^* - H_e)}$$

Therefore, when the flame zone is being created by the decreasing Damkohler number, the position of the maximum flame temperature depends on (aM_1) and (bM_2) rather than M_1 and M_2. Also, in that case[3], the position is determined for a given value of the above parameter through another numerically computed function. Hence, the sign of the above parameter does not necessarily reflect the direction to which the maximum temperature moves.

Finally, the maximum flame temperature is given by Eq. (64) to $O(\epsilon^{\frac{2}{a+b}})$. Eq. (64) first shows the expected result that a nonvanishing equilibrium constant reduces the maximum flame temperature. For those values of θ/H^* which would make the exponential term the predominant term of Eq. (64), the amount of the flame temperature drop increases as coefficients a and b are increased. Also, in that case, the actual order of the flame temperature drop as well as the flame zone thickness (see Eq. 62) is

$$O\left[\epsilon\ \exp\left(-\frac{\theta}{H^*}\right)\right]^{\frac{1}{a+b}}$$

In closing, it is pointed out here that it is understood in the evaluation of ζ_m and H_{im} that H^* is greater than H_e and H_{-e}. Otherwise, the maximum temperature is not created by the combustion and, therefore, ζ_m and H_{im} would have no meaning.

V. CONCLUDING REMARKS

The initial broadening of a diffusion flame sheet caused by an equilibrium constant becoming finite has been analyzed by the method of inner-and-outer expansions. The Damkohler number is assumed to be infinitely large and, therefore, the fluid is in local chemical equilibrium everywhere. Analytic expressions have been developed for the thickness of the flame zone, and the position and the value of the maximum flame temperature.

The various effects of the stoichiometric coefficients on the flame zone broadening have been discussed in detail in the preceding section. As a whole, it was found that varying the stoichometric coefficients affect the flame zone and the outer regions quite differently when the flame zone is created by a nonvanishing equilibrium constant compared to the case[3] where the zone was created by a decreasing Damkohler number. Also, the stoichiometric coefficient of the fuel affects the oxidant side more than the fuel side, and vice versa.

Now, the problems of diffusion flame sheet broadening due to either the decreasing Damkohler number or the nonvanishing equilibrium constant having been analyzed, the next problem worth considering may be the problem of simultaneous perturbation wherein both the Damkohler number and the equilibrium constant become perturbed from their respective limiting values.

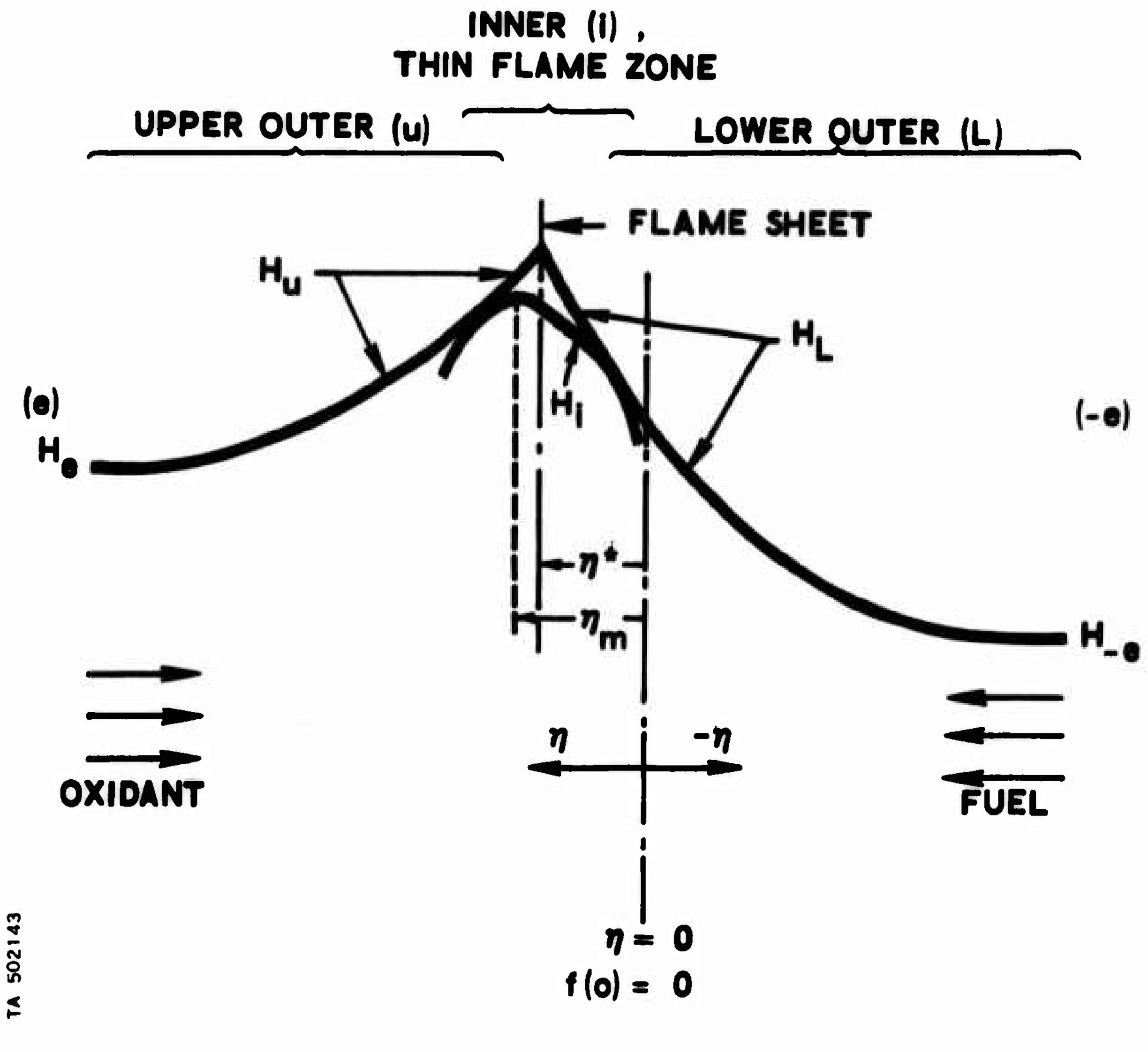

Figure 1. Sketch of Flame Sheet Broadening

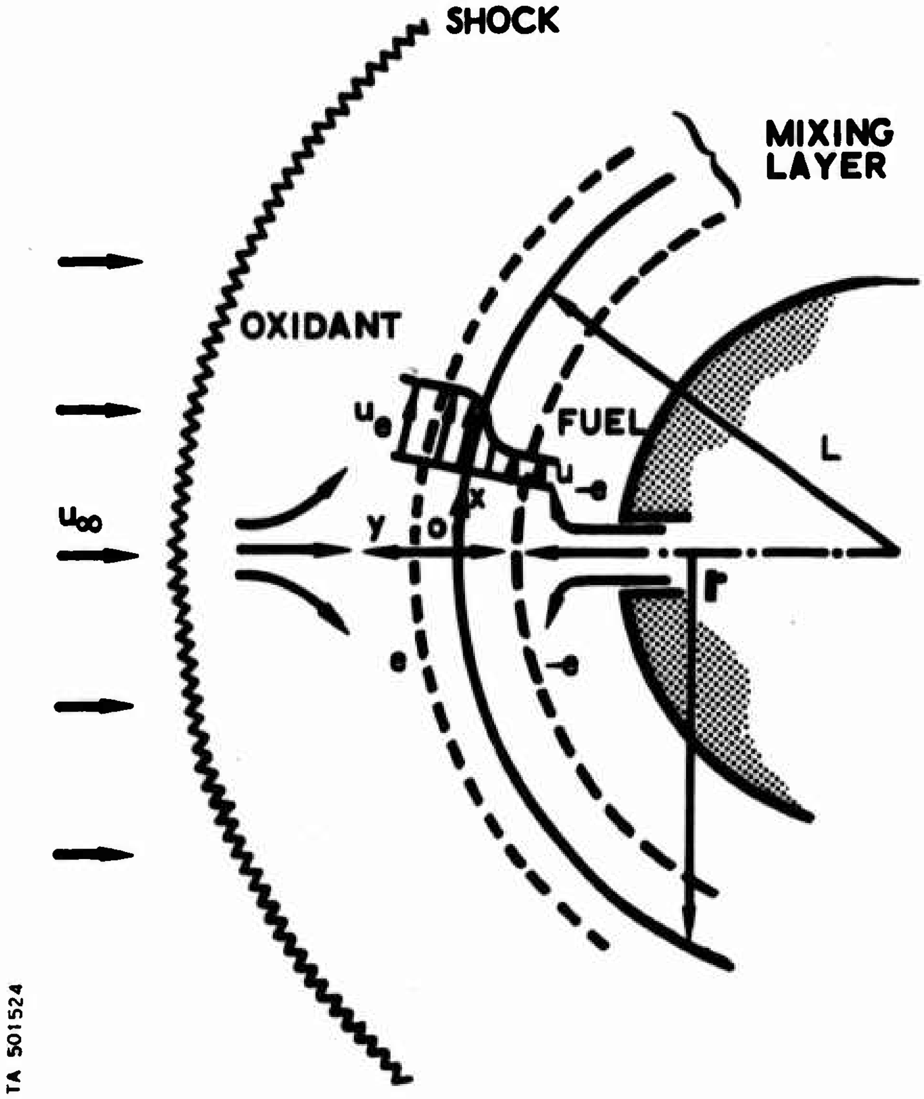

Figure 2. Flow Configuration

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SUPPLEMENTARY

INFORMATION

TAB No. 70-3

1 February 1970

IDENTIFICATION	FORMER STATEMENT	NEW STATEMENT	AUTHORITY
AD-477 791 Aerospace Corp., San Bernardino, Calif. Technical rept. Feb-Aug 65. Rept. no. TR- 69 (S6240-10)-1 Dec 65 Contract AF 0 (695)- 669	No Foreign without approval of Ballistic Systems Div., Attn: BSYDM, Norton AFB, Calif.	No limitation	SAMSO, USAF ltr, 24 Jul 69