

Cranfield Institute of Technology  
Department of Aerodynamics

Aero Note 1/74



CRANFIELD INSTITUTE OF TECHNOLOGY  
COLLEGE OF AERONAUTICS  
AERODYNAMICS DIVISION

DIFFUSION FLAMES ASSOCIATED WITH  
WEAK EXPLOSIONS

by

Maurice L. Rasmussen

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1403170574

Aero. Note 2/74.

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## ACKNOWLEDGEMENT

This work was done while the author was at the Cranfield Institute of Technology during Sabbatical Leave from the University of Oklahoma. The financial support of the Science Research Council is greatly appreciated. The general subject area of this work, diffusion flames, was proposed by Professor John Clarke who was a continuing source of knowledge and inspiration throughout this investigation. To the staff and students at Cranfield, the author owes his lasting gratitude for a year profitably spent, intellectually, culturally, and enjoyably.

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## SUMMARY

A general formulation for unsteady flows is set forth for which diffusion flames are regarded as discontinuity surfaces. A linearized theory is then developed for weak explosions associated with planar, cylindrical, and spherical symmetries. A simple combustion model for a ternary mixture of fuel, oxidant, and product species is utilized. The one-dimensional linearized shock-tube problem is analyzed in detail. Explicit results are obtained for the flame motion and the flame and flow-field development for arbitrary Prandtl number, Schmidt number, and second coefficient of viscosity. Wave fronts associated with the flame disturbance, initial pressure disturbance, and the value of the Prandtl number are delineated. The motion of a spherical flame associated with weak spherical explosions is analyzed and found ultimately to move toward the origin. The structure of the diffusion flame is analyzed by means of matched asymptotic expansions wherein the details of the flame structure are described by an "inner" expansion that is matched to the "outer" expansion that was obtained, to lowest order, with the flame treated as a discontinuity surface. Thus the variation of the flame structure with time is obtained for reaction broadening.

1. INTRODUCTION

When two combustible gases, an oxidant and a fuel, initially unmixed, are suddenly brought into contact with one another, a chemical reaction will ensue at the contact interface. The behaviour of the reaction will depend on a number of factors, such as the nature of the gases, the ambient temperature, the density of the gases, reaction rates, and features associated with the initiation of combustion. When the reaction is very intense and localized, the reaction region is referred to as a flame. In particular, it is referred to as a diffusion flame since the combustion is fed by processes of diffusion. The problems envisaged here are inherently unsteady and involve propagation of various disturbances arising from the flame itself as well as the initial conditions. Thus we are generally concerned with explosions, and those in particular that involve diffusion flames. Among a number of factors, we are interested in knowing, for instance, what temperature the flame obtains and how it varies with time. What are the disturbances caused by the flame and how do they propagate? How does the flame itself move? How does the flow field in general vary with time? Finding the answer to these and related questions is the subject of this investigation.

When the disturbances produced by the initial conditions as well as by the flame are large, the analysis required for the mathematical problem is of considerable difficulty. Indeed this is generally true for strong explosions even when there is no combustion involved. On the other hand, when the disturbances are small, a considerable amount of progress can be made. Happily enough, this limiting situation is of significant practical and



theoretical interest. Thus we shall utilize linearized theory and limit ourselves to diffusion flames in weak explosions.

It is consistent in this limit to deal with laminar flows and laminar diffusion flames.

Linearized theory has long been a mainstay in fluid-mechanics problems. It contains the embryonic behaviour of a good part of the more complete non-linear problem. As such it yields practical results and, often more importantly, leads to a deeper knowledge and insight of the more difficult complete problem. Some of its shortcomings can be dealt with by treatment of regions of nonuniformity. It often forms a foothold from which a stronger attack on the non-linear problem can be launched. A similar problem to the explosion problems treated herein, that of two gas streams uniting behind a solid cylinder and producing a diffusion flame, was examined by Clarke (1967a, 1967b) by means of linearized theory. This steady, two-dimensional problem is very akin to the shock-tube problem examined in this investigation. Application of linearized theory to nonequilibrium and chemically reacting flows has been developed and discussed by Clarke and McChesney (1964), Vincenti and Kruger (1965), and Clarke (1969). A recent paper by Wu and Turner (1974) also elaborates on the linear theory. A paper by Sforza and Bloom (1965) bears a remote connection to the explosion problems considered here.

Although diffusion flames associated with steady flows have been widely investigated, intrinsically unsteady flows have not met with the same interest or thoroughness. Clarke and Stegen (1968) investigated some unsteady behaviours of diffusion-flame sheets. Their investigation considered perturbations to a basic

two-dimensional flame and flow field. In the present analysis we consider intrinsically unsteady flows associated with weak explosions. The basic problem to be considered is that of the one-dimensional shock-tube problem, wherein a fuel and product mixture are separated initially from an oxidant and product mixture by a diaphragm. At a given instant the diaphragm disappears, and the subsequent motion and combustion flame are to be determined. The outer problem wherein the flame is replaced by a discontinuity surface is analyzed by means of linearized theory. Aside from this approximation and the utilization of simple fuel, oxidant, and product ternary mixture, there are a minimum of other major restrictions. The Prandtl number and Schmidt number are left arbitrary and the second coefficient of viscosity is retained as an arbitrary value. A number of general results are established and explicit expressions for large time are obtained. The initial motion of a spherical flame associated with weak spherical explosions is also obtained.

After the flow field associated with the flame discontinuity surface has been determined, the structure of the flame is then investigated by regarding it as the companion "inner" problem in a scheme of matched asymptotic expansions. The "outer" problem is thus recognized as the flow field associated with the flame treated as a Burke-Schumann discontinuity sheet. Details of the structure of the flame and its variation with time are thus obtained for reaction broadening.

This investigation begins with some generality in the formulation of unsteady-flow problems containing diffusion flames. This is desirable since the general conditions holding across an unsteady

diffusion flame sheet appear not to have been explicitly stated, except perhaps by Clarke and Stegen (1968) in the context of their own investigation. A number of general results associated with conservation of species, mass, momentum, and energy are derived without specification of particular constitutive relations. The constitutive relations associated with the Navier-Stokes approximation are utilized as a special case. Thus, with specification of appropriate constitutive relations, problems involving non-Newtonian flows may be treated directly in future investigations by utilization of the general results derived here. In this connection, constitutive relations for the heat-flux and diffusion-flux vectors are derived by methods of continuum mechanics. Such a methodology could prove useful for non-Newtonian problems where results from kinetic theory are not readily obtained or directly applicable.

## 2. GENERAL FORMULATION OF THE PROBLEM

### 2.1 Basic Equations

The fundamental equations of change for mass, species, momentum, and energy for a gaseous mixture of  $n$  reacting species are

$$\frac{D\rho}{Dt} + \rho \operatorname{div} \vec{v} = 0 \quad (2.1)$$

$$\rho \frac{Dc_\alpha}{Dt} = - \operatorname{div} \vec{j}_\alpha + \rho K_\alpha \quad (2.2)$$

$$\rho \frac{D\vec{v}}{Dt} = - \nabla p + \operatorname{div} \vec{\tau} \quad (2.3)$$

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \vec{\tau} : \vec{E} - \operatorname{div} \vec{q} \quad (2.4)$$

where  $\rho$  is the mass density,  $\vec{v}$  the mass mean velocity vector,  $c_\alpha$  the mass fraction of species  $\alpha$ ,  $\vec{j}_\alpha$  the diffusion-flux vector for species  $\alpha$ ,  $K_\alpha$  the species mass production rate per unit mass,  $p$  the pressure,  $\vec{\tau}$  the viscous stress tensor,  $\vec{E}$  the rate of strain tensor,  $h$  the enthalpy, and  $\vec{q}$  the heat-flux vector. The species terms  $c_\alpha$ ,  $\vec{j}_\alpha$ , and  $K_\alpha$  satisfy the relations

$$\sum_{\alpha=1}^n c_\alpha = 1 \quad (2.5)$$

$$\sum_{\alpha=1}^n \vec{f}_{\alpha} = 0 \quad (2.6)$$

$$\sum_{\alpha=1}^n K_{\alpha} = 0 \quad (2.7)$$

and hence are not all independent. Body forces have been omitted.

## 2.2 Constitutive Relations

We assume the stress-rate-of-strain relations are given by the Navier-Stokes relations

$$\vec{\tau} = 2\mu \vec{E} + \lambda (\text{div } \vec{v}) \vec{I} \quad (2.8)$$

$$\vec{E} \equiv \frac{1}{2} [ \nabla \vec{v} + (\nabla \vec{v})^t ] \quad (2.9)$$

where  $\mu$  and  $\lambda$  are the first and second coefficients of viscosity, restricted by  $\mu > 0$  and  $(\lambda + \frac{2}{3}\mu) \geq 0$ . Consistent with these relations, we assume that the diffusion-flux and heat-flux vectors are given by

$$\vec{f}_{\alpha} = - \sum_{\beta=1}^{n-1} \tilde{D}_{\alpha\beta} \nabla C_{\beta} - D_{\alpha}^{(p)} \nabla h_{\alpha} p - D_{\alpha}^{(T)} \nabla h_{\alpha} T, \quad (2.10)$$

$\alpha = 1, 2, \dots, n-1$

$$\vec{q} = -k \nabla T + \sum_{\alpha=1}^{n-1} \left( \frac{\partial h}{\partial C_{\alpha}} \right)_{p, T, C_{\beta}} \vec{f}_{\alpha} + \sum_{\alpha, \beta=1}^{n-1} A_{\alpha\beta}^{-1} D_{\beta}^{(T)} \vec{f}_{\alpha} \quad (2.11)$$

Only the first  $n-1$  variables  $C_{\alpha}$  and  $\vec{f}_{\alpha}$  are regarded as independent here, the variables  $C_n$  and  $\vec{f}_n$  being determined from (2.5) and

(2.6). Equations (2.10) and (2.11) can be derived from kinetic

theory by means of the Chapman-Enskog expansion for the Boltzmann equations (see Hirshfelder, Curtiss, and Bird 1954). They also can be established from principles of continuum mechanics. Since this technique is not widely known in gas dynamics, a derivation from this point of view is given in Appendix A. The multi-component diffusion coefficients are denoted by  $\tilde{D}_{\alpha\beta}$ , only some of which are independent, as delineated in Appendix A. The pressure-diffusion coefficients  $D_{\alpha}^{(p)}$  and the coefficients  $A_{\alpha\beta}^{-1}$  are functions of  $\tilde{D}_{\alpha\beta}$ , also delineated in Appendix A. The first  $n-1$  thermal-diffusion coefficients  $D_{\alpha}^{(T)}$  are independent, the  $n$ th coefficient being determined consistently with (2.6).

The thermal conductivity is denoted by  $k$  and is positive.

The coefficients  $\tilde{D}_{\alpha\beta}$ ,  $D_{\alpha}^{(T)}$ , and  $k$ , as well as the first and second coefficients of viscosity,  $\mu$  and  $\lambda$ , can be evaluated by means of kinetic theory when particular molecular interactions are specified. For our purposes here, we regard these coefficients as phenomenological, to be evaluated empirically or by kinetic theory.

To close the system of equations, we need to add thermal and caloric equations of state in the forms

$$p = p(p, T, c_1, c_2, \dots, c_{n-1}) \quad (2.12)$$

$$h = h(p, T, c_1, c_2, \dots, c_{n-1}) \quad (2.13)$$

In addition we need specific expressions for the species source terms  $K_\alpha$ . We shall defer this till later when we consider a special simple chemical reaction.

### 2.3 Conditions Across a Diffusion-Flame Discontinuity.

We now want to treat a diffusion flame as a surface of discontinuity, somewhat akin to the treatment of Clarke (1967a). The jump conditions across an arbitrary surface of discontinuity are well known for mass, momentum, and energy. Let the subscripts 1 and 2 denote conditions on either side of a surface of discontinuity, and let  $\vec{V}$  and  $\hat{n}$  be the velocity and unit normal of a point on the surface of discontinuity. By the analysis of Eringen (1967), for instance, we can obtain the jump conditions for mass, momentum, and energy as

$$\rho_1 (\vec{V}_1 - \vec{S}) \cdot \hat{n} = \rho_2 (\vec{V}_2 - \vec{S}) \cdot \hat{n} \equiv m \quad (2.14)$$

$$m (\vec{V}_1 - \vec{S}) + \rho_1 \hat{n} - \hat{n} \cdot \vec{T}_1 = m (\vec{V}_2 - \vec{S}) + \rho_2 \hat{n} - \hat{n} \cdot \vec{T}_2 \quad (2.15)$$

$$m \left[ h_1 + \frac{1}{2} (\vec{V}_1 - \vec{S})^2 \right] - \hat{n} \cdot \vec{T}_1 \cdot (\vec{V}_1 - \vec{S}) + \vec{q}_1 \cdot \hat{n} = m \left[ h_2 + \frac{1}{2} (\vec{V}_2 - \vec{S})^2 \right] - \hat{n} \cdot \vec{T}_2 \cdot (\vec{V}_2 - \vec{S}) + \vec{q}_2 \cdot \hat{n} \quad (2.16)$$

If we now assume, along with Clarke (1967a), that the flow variables  $\rho$ ,  $p$ ,  $h$ ,  $\tau$ ,  $C_\alpha$ , and  $\vec{V}$  are continuous across the flame discontinuity, then (2.14) is identically

satisfied. It follows from the momentum equation (2.15) that the stress vector is continuous across the flame discontinuity;

$$\hat{n} \cdot \vec{\tau}_1 = \hat{n} \cdot \vec{\tau}_2 \quad (2.17)$$

The energy equation (2.16) yields that the normal component of the heat-flux vector is continuous across the flame sheet:

$$\vec{q}_1 \cdot \hat{n} = \vec{q}_2 \cdot \hat{n} \quad (2.18)$$

Relations (2.17) and (2.18) are quite general and do not depend on the nature of the constitutive equations. When the constitutive relations (2.10) and (2.11) are admitted, then (2.18) leads to a jump relation between the normal components of temperature, pressure, and concentration gradients.

We still have to establish a jump condition appropriate for the equation of change of species. To do this we must examine the nature of the source terms,  $K_d$ , as they pertain to a diffusion flame. The essence of a diffusion flame is that it separates two species that diffuse into the flame and produce an intense chemical reaction. The flame moves in such a way that the two species are annihilated by the flame and one or more new species are produced as a result of the chemical reaction. As Clarke (1967a) spells out, the pertinent chemical reaction that produces the diffusion flame is characterized by two reaction times, a forward reaction time,  $\tau_f$ , and a reverse reaction time,  $\tau_r$ . Because of the intense behavior of the flame,  $\tau_f$  is very small and  $\tau_r$  is very large. In the limiting situation



we take  $\mathcal{L}_f \rightarrow 0$  and  $\mathcal{L}_r \rightarrow \infty$ . On the other hand,  $K_d$  pertaining to the species participating in the chemical reaction producing the diffusion flame will be zero on either side of the flame since one or the other species required for the reaction is not present. At the diffusion flame itself, the two species combine and produce an intense reaction since  $\mathcal{L}_f \rightarrow 0$ . In this limit the flame can be regarded as a discontinuity surface. In a fashion akin to that of Clarke (1967a) we now regard  $K_d$  as made up of two parts and write

$$K_d = K_d + S_d \delta(z_n) \quad (2.19)$$

Here  $K_d$  represents all the reactions not associated with the flame discontinuity and  $S_d \delta(z_n)$  represents those associated with the diffusion flame. The function  $\delta(z_n)$  is a Dirac delta function and  $z_n$  is a coordinate measured normal from the flame discontinuity and equal to zero on the discontinuity surface. The variable  $S_d$  is the flame strength of the flame and may vary from point to point on the flame surface, as well as with time. The function  $K_d$  is assumed to be free of any intense localized behaviours associated with flame discontinuities.

Because of the properties of the Dirac delta function, any finite volume integral of  $\rho S_d \delta(z_n)$  over a region  $R$  that includes a portion of the diffusion flame can be expressed as a surface integral

$$\iiint_R \rho S_d \delta(z_n) dV = \iint_{S_F} \rho S_d dS \quad (2.20)$$

over the enclosed flame surface  $S_F$ . We can now apply this result to the integral equation governing the change of mass of species  $\alpha$  in the region  $R$ . We have

$$\frac{D}{Dt} \iiint_R \rho c_\alpha dV = - \oint_S \vec{j}_\alpha \cdot \hat{n} dS + \iiint_R \rho K_\alpha dV \quad (2.21)$$

where  $S$  is the surface that encloses  $R$ .

We now shrink the region  $R$  so that it embraces the flame surface  $S_F$ . Since  $\rho$  and  $c_\alpha$  are regarded as continuous, the left-hand integral vanishes when the volume is reduced to zero, as does the volume integral over  $\rho K_\alpha$ . The diffusion-flux vector, however, is allowed to be discontinuous, and since  $S_F$  is arbitrary, we obtain the jump conditions for  $\vec{j}_\alpha$  to be

$$\vec{j}_{\alpha 2} \cdot \hat{n} = \vec{j}_{\alpha 1} \cdot \hat{n} + \rho_F S_\alpha \quad (2.22)$$

where  $\hat{n}$  is the unit normal that points from side 1 towards side 2 of the flame discontinuity, and  $\rho_F$  is the value of the density on the flame sheet. Thus the jump in the normal component of the diffusion-flux vector is equal to the strength of the flame sheet. Again (2.22) is a general result and does not depend on the constitutive relation for the diffusion-flux vector.\*

Because the two species that participate in the diffusion-flame reaction are continuous and vanish on one side of the flame or the other, it follows that the mass fractions of these two species, say  $C_X$  and  $C_F$ , must vanish on the flame sheet:

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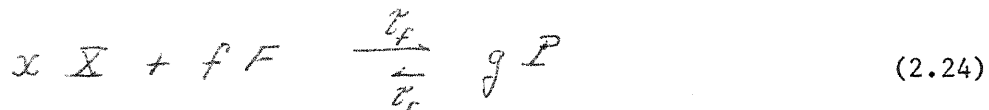
\*Eq. (2.22) holds across each flame sheet that exists. The remainder of the discussion assumes there is only a single flame sheet.

$$C_X = C_F = 0 \quad \text{on the flame sheet,} \quad (2.23)$$

Thus (2.18), (2.22), and (2.23) are to be imposed as boundary conditions at the flame sheet. The flame strength  $S_d$  and the position of the flame are to be found as part of the solution. It is interesting to note that  $S_d$  has the dimensions of speed.

#### 2.4 Simple Fuel-Oxidant Combustion Model

In this investigation we wish to fix our attention on the interaction of diffusion flame and the gas dynamics of weak disturbances. Along with Clarke (1967a), therefore, we fix our attention on a simple single reaction process described by



where  $X$ ,  $F$ , and  $P$  represent oxidant, fuel, and product species, and  $x$ ,  $f$ , and  $g$  represent the respective stoichiometric coefficients. The reaction rates for this case are

$$\begin{aligned} K_X &= -x W_X \left[ \frac{C_X^x C_F^f}{\nu_f} - \frac{C_P^g}{\nu_r} \right] \\ K_F &= -f W_F \left[ \frac{C_X^x C_F^f}{\nu_f} - \frac{C_P^g}{\nu_r} \right] \\ K_P &= g W_P \left[ \frac{C_X^x C_F^f}{\nu_f} - \frac{C_P^g}{\nu_r} \right] \end{aligned} \quad (2.25)$$

where  $W_X$ ,  $W_F$ , and  $W_P$  are the molecular weights of the

oxidant, fuel, and product species. When the diffusion flame is regarded as a discontinuity surface then  $\zeta_f \rightarrow 0$ ,  $\zeta_r \rightarrow \infty$ , and since either  $C_X$  or  $C_F$  is zero, except on the flame surface itself, the appropriate limiting approximations are

$$K_X = - \alpha W_X S' \delta(z_n)$$

$$K_F = - f W_F S' \delta(z_n) \tag{2.26}$$

$$K_P = g W_P S' \delta(z_n)$$

where  $S_X = - \alpha W_X S'$ ,  $S_F = - f W_F S'$ , and  $S_P = g W_P S'$ .

Here the function  $S'$  is the strength of the flame, which may vary with time and with position on the flame sheet. For this situation the function  $K_{ed}$  in (2.19) is zero.

Even though there are three species in this model, we essentially have to deal with binary mixtures on either side of the flame discontinuity since either the fuel or oxidant species is absent. This leads to a considerable simplification in the analysis of these kinds of problems.

## 2.5 Alternative Form of the Energy Equation

It is useful to rewrite the energy equation (2.4) in terms of the temperature instead of enthalpy. To do this we eliminate the enthalpy by means of the caloric equation of state (2.13).

We then obtain

$$\rho c_p \frac{DT}{Dt} = \left[ 1 - \rho \left( \frac{\partial h}{\partial p} \right)_{T, c_d} \right] \frac{Dp}{Dt} + \vec{v} \cdot \vec{e} - \sum_{\alpha=1}^{n-1} \vec{f}_\alpha \cdot \vec{v} \left( \frac{\partial h}{\partial c_\alpha} \right)_{p, T, c_\beta}$$

$$- \sum_{\alpha=1}^{n-1} \left( \frac{\partial h}{\partial c_\alpha} \right)_{p, T, c_\beta} R_{\alpha d}$$

$$- \text{div} \left[ \vec{q} - \sum_{\alpha=1}^{n-1} \left( \frac{\partial h}{\partial c_\alpha} \right)_{p, T, c_\beta} \vec{f}_\alpha \right] \tag{2.27}$$

where

$$c_p \equiv \left( \frac{\partial h}{\partial T} \right)_{p, c_d}$$

The first term on the right is associated with work done on a fluid element by the pressure forces in compression or expansion of the fluid. The last term is a flux term associated with energies crossing the boundary of a fluid element. The second, third, and fourth terms are apparent sources of temperature arising from viscous dissipation, diffusion, and chemical reactions. The apparent sources of temperature arising from viscous dissipation and diffusion are nonlinear and will disappear in a linearized approximation, leaving only the linearized version of the fourth term as an apparent temperature source, or heat-of-reaction. For a mixture of thermally perfect gases, the term  $\left( \frac{\partial h}{\partial p} \right)_{T, c_d}$  vanishes, but this does not provide any essential simplification in a linearized theory.

3. LINEARIZED UNSTEADY FLOW

3.1 Basic Assumptions and Definitions

We now consider a basic ambient state made up entirely of a product gas with pressure, density, and temperature denoted by  $p_0$ ,  $\rho_0$ , and  $T_0$ . The speed of sound for this ambient state is denoted by  $a_0$ . We introduce nondimensional primed perturbation variables defined by

$$\begin{aligned}
 p &= p_0 (1 + p') \\
 \rho &= \rho_0 (1 + \rho') \\
 T &= T_0 (1 + T') \\
 c_x &= c_x' \\
 c_F &= c_F' \\
 c_P &= 1 + c_P' \\
 \vec{V} &= a_0 \vec{V}'
 \end{aligned}
 \tag{3.1}$$

We further assume that the mixture behaves as a combination of perfect gases. It follows that

$$\begin{aligned}
 c_p &\equiv \left( \frac{\partial h}{\partial T} \right)_{p, c_d} = c_x' c_{p_x} + c_F' c_{p_F} + (1 + c_P') c_{p_P} \\
 \left( \frac{\partial h}{\partial p} \right)_{T, c_d} &= 0
 \end{aligned}
 \tag{3.2}$$

$$\left( \frac{\partial h}{\partial c_d} \right)_{p, T, c_B} = h_d(T) - h_P(T)$$

where we have taken  $C_1 = \frac{C}{X}$ ,  $C_2 = C_F$ , and  $C_3 = C_D$ . We also have  $a_0^2 = \gamma p_0 / \rho_0$ , where  $\gamma$  is the ratio of specific heats for the product gas. *We identify  $a_0$  as the frozen sound speed.* Further we normalize the time and space variables such that

$$\begin{aligned} \tau &\equiv \frac{\rho_0 a_0^2}{\tilde{\mu}_0} t \\ \bar{r} &\equiv \frac{\rho_0 a_0}{\tilde{\mu}_0} \bar{r} \end{aligned} \quad (3.3)$$

where  $\tilde{\mu}_0 \equiv 2\mu_0 + \lambda_0$  is the reduced or effective viscosity. The "barred" space variables are dimensional and the unbarred are dimensionless. The dimensionless "del" operator is denoted by  $\bar{\nabla} \equiv \frac{\partial}{\partial \bar{r}}$ .

Because a binary mixture prevails on either side of the diffusion flame, the diffusion-flux vectors for the oxidant and fuel species can be written

$$\begin{aligned} \bar{J}_X &= -\tilde{D}_{XP} \bar{\nabla} C_X - D_X^{(P)} \bar{\nabla} \ln p - D_X^{(T)} \bar{\nabla} \ln T \\ \bar{J}_F &= -\tilde{D}_{FP} \bar{\nabla} C_F - D_F^{(P)} \bar{\nabla} \ln p - D_F^{(T)} \bar{\nabla} \ln T \end{aligned} \quad (3.4)$$

As shown in Appendix A, or by kinetic theory, the pressure-diffusion coefficients and thermal-diffusion coefficients vanish when their corresponding mass fractions,  $C_X$  or  $C_F$ , vanish. Thus when the ambient medium does not contain any oxidant or fuel species, the perturbation contribution arising from the pressure-diffusion and thermal-diffusion terms are non-linear and can be neglected

in a linearized theory. In this case, therefore, Fick's law prevails, and we have for the linearized case

$$\begin{aligned} \vec{J}_X &= -\tilde{D}_{XP_0} \vec{\nabla} c'_X \\ \vec{J}_F &= -\tilde{D}_{FP_0} \vec{\nabla} c'_F \end{aligned} \quad (3.5)$$

Along with Clarke (1967a) we further assume, for the sake of simplicity, that the binary diffusion coefficients for oxidant-product and fuel-product diffusion are equal, that is,

$$\tilde{D}_{XP_0} = \tilde{D}_{FP_0} = D_0 \quad (3.6)$$

Correspondingly, the Dufour effect in the heat-flux vector gives rise to a non-linear contribution when the fuel and oxidant are not present in the basic ambient conditions. The appropriate linearized version <sup>of  $\vec{\psi}$</sup>  is thus

$$\vec{q} = -k_0 \vec{\nabla} T + (h_{X_0} - h_{P_0}) \vec{J}_X + (h_{F_0} - h_{P_0}) \vec{J}_F \quad (3.7)$$

Non-dimensional variables associated with the diffusion-flux and heat-flux vectors are the Prandtl and Schmidt numbers:

$$\begin{aligned} Pr &\equiv \frac{\tilde{\mu}_0 c_{p_0}}{k_0} \\ Sc &\equiv \frac{\tilde{\mu}_0}{D_0} \end{aligned} \quad (3.8)$$



Finally a nondimensional effective heat of reaction,  $Q$ , can be defined as

$$Q \equiv \frac{xW_I (h_{I_0} - h_{P_0}) + fW_F (h_{F_0} - h_{P_0})}{C_{p_0} T_0} \quad (3.9)$$

and a nondimensional flame strength as

$$\tilde{S} \equiv \frac{S'}{a_0} \quad (3.10)$$

### 3.2 Linearized Equations

The nondimensional linearized versions of the mass, species, momentum, and temperature-energy equations, appropriate for diffusion flames discussed in the previous section, are

$$\frac{\partial p'}{\partial \tau} + \nabla \cdot \vec{v}' = 0 \quad (3.11)$$

$$\frac{\partial c'_I}{\partial \tau} = \frac{1}{Sc} \nabla^2 c'_I - xW_I \tilde{S} \delta(z_n) \quad (3.12)$$

$$\frac{\partial c'_F}{\partial \tau} = \frac{1}{Sc} \nabla^2 c'_F - fW_F \tilde{S} \delta(z_n) \quad (3.13)$$

$$\frac{\partial \vec{v}'}{\partial \tau} = -\frac{1}{\delta} \nabla p' + \nabla(\nabla \cdot \vec{v}') - \frac{\mu_0}{\mu_0} \nabla \times (\nabla \times \vec{v}') \quad (3.14)$$

$$\frac{\partial T'}{\partial \tau} = \frac{\delta-1}{\delta} \frac{\partial p'}{\partial \tau} + \frac{1}{Pr} \nabla^2 T' + Q \tilde{S} \delta(z_n) \quad (3.15)$$

The linearized perturbation equation for the thermal equation of state, for a ternary mixture of thermally perfect gases, can be written

$$p' = p' + T' + \alpha_X c'_X + \alpha_F c'_F \quad , \quad (3.16)$$

where

$$\alpha_X \equiv \frac{R_X}{R_P} - 1 \quad (3.17a)$$

$$\alpha_F \equiv \frac{R_F}{R_P} - 1 \quad , \quad (3.17b)$$

and  $R_X$ ,  $R_F$ , and  $R_P$  are specific gas constants. Use was made of the relation

$$c'_X + c'_F + c'_P = 0 \quad , \quad (3.18)$$

which is the perturbation counterpart of (2.5).

When the flame sheet vanishes,  $\tilde{S}' = 0$ , and when there is only one species,  $c'_X = c'_F = 0$ , the above equations reduce to those studied previously by Rasmussen and Lake (1973), as well as others.

### 3.3 Potential Flow

In the general problem, the velocity vector can be divided into rotational and irrotational parts (see Eringen 1967).

Here we shall concern ourselves with those problems that are irrotational. These kind of problems will usually be one-dimensional or with cylindrical or spherical symmetry such that  $\text{curl } \vec{v}'$  identically vanishes. For these irrotational flows, we write

$$\vec{v}' = \nabla \phi \quad , \quad (3.19)$$

where  $\phi$  is a dimensionless (scalar) velocity potential.

We can now integrate the momentum equation (3.14) once and obtain for the pressure perturbation

$$p' = \gamma (\nabla^2 \phi - \rho_0 \phi) \quad . \quad (3.20)$$

Notice for irrotational flows the first and second coefficients of viscosity always appear in the combination  $\tilde{\mu}_0 \equiv 2\mu_0 + \lambda_0$ .

The continuity equation (3.11) can now be written

$$\rho_0' + \nabla^2 \phi = 0 \quad (3.21)$$

With the introduction of the velocity potential the problem becomes considerably simplified.

#### 3.4 Reduction of the Differential Equations

It is not necessary to obtain a single differential equation for any one of the flow variables, but it is useful

and enlightening to do so. We begin by introducing the thermal diffusion operator,  $\mathcal{D}_P$ , defined as

$$\mathcal{D}_P \equiv \frac{\partial}{\partial z} - \frac{1}{L_r} \nabla^2 \quad (3.22)$$

Differentiating equation (3.16) first with time and then with  $\mathcal{D}_P$  and then eliminating the temperature by means of equation (3.15), we obtain

$$\begin{aligned} \frac{\delta-1}{\delta} \rho'_{zz} - \mathcal{D}_P (\rho'_z - \rho'_z) &= \left( \frac{S_c}{L_r} - 1 \right) \left[ d_I c'_I + d_F c'_F \right]_{zz} \\ + \frac{S_c}{L_r} \tilde{S} (d_I \alpha W_I + d_F \alpha W_F) \delta_p(z_n) &- Q \tilde{S} \mathcal{D}_P \delta_p(z_n) \end{aligned} \quad (3.23)$$

After expanding the left-hand side of this equation by means of equations (3.20) and (3.21), we have

$$\begin{aligned} \delta \nabla^4 \phi + \nabla^4 \phi - (\delta + L_r) \nabla^2 \phi_{zz} + L_r (\phi_{zz} - \nabla^2 \phi)_{zz} &= \\ (S_c - L_r) [d_I c'_I + d_F c'_F]_{zz} & \\ + S_c \tilde{S} (d_I \alpha W_I + d_F \alpha W_F) \delta_p(z_n) - L_r \tilde{S} Q \mathcal{D}_P \delta_p(z_n) & \end{aligned} \quad (3.24)$$

This equation, with the right-hand side equal to zero, was utilized by Bienkowski (1965) and by Rasmussen and Lake (1973).

The presence of the terms  $c'_{Izz}$  and  $c'_{Fzz}$  on the right-hand side of equation (3.24) represents the effect of diffusion. The derivatives of the Dirac delta function represent the discontinuity associated with the flame sheet; on either

side of the flame sheet the derivatives of  $\delta$ , as well as  $\delta$  itself, vanish. Equation (3.24) can then be written in simpler form as

$$\delta \nabla^4 \Phi + \nabla^4 \Phi - (\delta + L_r) \nabla^2 \Phi_{rr} + L_r (\Phi_{tt} - \nabla^2 \Phi)_{tt} = (\delta_c - L_r) \left[ \beta_I C'_I + \beta_F C'_F \right] \delta \rho \quad (3.25)$$

which holds on either side of the flame sheet.

It is useful to deal with equations (3.24) or (3.25) in their inhomogeneous forms because  $C'_X$  and  $C'_F$  can be determined separately since the diffusion equations (3.12) and (3.13), together with their initial and boundary conditions, are uncoupled from the other equations. We should note, however, that  $C'_X$  and  $C'_F$  can be eliminated from equation (3.23) by operating on it with the mass-diffusion operator,  $D_S$ , defined as

$$D_S \equiv \frac{\partial}{\partial t} - \frac{1}{S_c} \nabla^2 \quad (3.26)$$

The equation thus obtained is a seventh-order equation for  $\Phi$  with the right-hand side involving only derivatives of delta functions, which vanish on either side of the flame sheet.

Identical seventh-order equations, but with different combinations of delta functions on the right-hand sides, can be obtained for the state variables  $f'$ ,  $p'$ , and  $T'$ .

When  $L_r = S_c$ , that is, when the Lewis number is unity,

the right side of (3.25) vanishes on either side of the flame sheet. In this case the governing equations for  $\phi'$ , as well as for  $f'$ ,  $\rho'$ , and  $T'$ , are fifth order and are the same as the equations studied by Bienkowski (1965) and Rasmussen and Lake (1973) for homogeneous media.

### 3.5 Boundary Conditions on the Flame Sheet.

For the simple irrotational flows considered here, let  $X$  represent the Cartesian coordinate in one dimensional flow or the polar coordinate for flows with cylindrical or spherical symmetry. Then the coordinate normal to the flame sheet can be written as

$$z_n = X - x_s(t) \quad , \quad (3.27)$$

where  $x_s(t)$  is the position of the flame sheet as a function of time. Let the unit normal to the flame sheet point in the direction of increasing  $X$ . Then the jump condition (2.22) along with the condition  $C'_x = C'_F = 0$  on  $X = x_s$  leads to the relations

$$\left[ \frac{\partial C'_x}{\partial X} \right]_{x_s^-}^{x_s^+} = \alpha W_x S'_c \tilde{S}'^2$$

$$\left[ \frac{\partial C'_F}{\partial X} \right]_{x_s^-}^{x_s^+} = f W_F S'_c \tilde{S}'^2 \quad (3.28)$$

where the bracket notation indicates the change in the variable enclosed by the brackets between the limits shown. Because

the gradients of  $C'_I$  and  $C'_F$  vanish on opposite sides of the flame sheet, we can eliminate the flame strength in equations (3.28) and obtain

$$\frac{\partial C'_I}{\partial x}(x_s(t), t) = - \frac{2W_I}{FW_F} \frac{\partial C'_F}{\partial x}(x_s(t), t) \quad (3.29)$$

After  $C'_I$  and  $C'_F$  have been determined by means of this boundary condition, as well as the flame position  $x_s(t)$ , the flame strength,  $\tilde{S}^n$ , is then determined from (3.28).

The jump condition (2.18), together with (2.22) and (3.7), leads to the following jump condition on the temperature gradient:

$$\left[ \frac{\partial T}{\partial x} \right]_{x_s^-}^{x_s^+} = - P_r G \tilde{S}^n(t) \quad (3.30)$$

The right-hand side is known when the flame strength,  $\tilde{S}^n(t)$ , has been determined from the uncoupled diffusion problem.

Note that the thermal-diffusion coefficients  $D_I^{(T)}$  and  $D_F^{(T)}$  will not enter the flame temperature jump condition even in the nonlinear problem because  $D_I^{(T)}$  and  $D_F^{(T)}$  vanish on the flame owing to the conditions  $C_I = C_F = 0$  on  $x = x_s$ .

The flame boundary conditions shown here are entirely akin to those set up by Clarke (1967a,b). The governing differential equations for the present unsteady flow problems to be considered are different from the linearized equations utilized for the planar steady flow problems studied by Clarke.

With the formulation of the linearized theory now complete, we wish to study the one-dimensional shock-tube problem in some detail. We shall also examine some of the flame properties for weak spherical explosions after that.

#### 4. LINEARIZED SHOCK-TUBE PROBLEM

##### 4.1 Description and Initial Conditions.

Consider a planar diaphragm at  $X=0$  that initially separates two semi-infinite regions. On the right-hand side of the diaphragm,  $X>0$ , let there be a mixture of product gas and a small amount of fuel gas. On the left-hand,  $X<0$ , let there be a mixture of product gas and a small amount of oxidant gas. Further, let the temperature and pressure on the left-hand side vary by small amounts from the prevailing ambient conditions on the right-hand side. At the instant  $t=0$ , the diaphragm instantaneously disappears. We assume that the ambient temperature and density,  $T_0$  and  $\rho_0$ , are sufficiently high that combustion is spontaneously initiated. We wish to determine the flow field that develops because of the removal of the diaphragm. The initial conditions are depicted in Sketch 1.



Oxidant side

Fuel side

$$\underline{X < 0, t < 0}$$

$$\rho' = \Delta \rho$$

$$p' = \Delta p$$

$$T' = \Delta T$$

$$C'_X = \Delta X$$

$$C'_F = 0$$

$$\underline{X > 0, t < 0}$$

$$\rho' = 0$$

$$p' = -d_F \Delta_F$$

$$T' = 0$$

$$C'_X = 0$$

$$C'_F = \Delta_F$$

$$\Delta p = \Delta \rho + \Delta T + d_X \Delta X$$

Sketch 1. Initial Configuration and Conditions.

The initial values  $\Delta \rho$ ,  $\Delta p$ ,  $\Delta T$ , and  $\Delta X$  are not all independent, but are related as indicated in Sketch 1.

4.2 Flame Properties and Species Concentrations.

The problem for the species concentrations is uncoupled from the other equations. The pertinent characteristic length involved is the displacement of the flame sheet itself,  $X_S(\tau)$ , and we seek a solution by making the following change of variable:

$$\eta = \frac{x}{X_S(\tau)}, \quad c' = \tilde{c}'(\eta, \tau) \tag{4.1}$$

The differential equations (3.12) and (3.13) and the flame boundary conditions become

$$x_3^2 \frac{\partial \overset{N'}{\mathcal{L}}_E}{\partial t} = \eta x_3 \frac{dx_3}{dt} \frac{\partial \overset{N'}{\mathcal{L}}_E}{\partial \eta} + \frac{1}{S_c} \frac{\partial \overset{N'}{\mathcal{L}}_E}{\partial \eta^2}, \quad x < x_3$$

$$x_3^2 \frac{\partial \overset{N'}{\mathcal{L}}_F}{\partial t} = \eta x_3 \frac{dx_3}{dt} \frac{\partial \overset{N'}{\mathcal{L}}_F}{\partial \eta} + \frac{1}{S_c} \frac{\partial \overset{N'}{\mathcal{L}}_F}{\partial \eta^2}, \quad x > x_3 \quad (4.2)$$

$$\overset{N'}{\mathcal{L}}_E(1, t) = \overset{N'}{\mathcal{L}}_F(1, t) = 0 \quad (4.3)$$

$$\frac{\partial \overset{N'}{\mathcal{L}}_E}{\partial \eta}(1, t) = - \frac{2W_E}{FW_F} \frac{\partial \overset{N'}{\mathcal{L}}_F}{\partial \eta}(1, t) \quad (4.4)$$

The initial conditions, of course, are

$$\begin{aligned} \overset{N'}{\mathcal{L}}_E(x, 0) &= \Delta_E, & x < x_3 \\ \overset{N'}{\mathcal{L}}_F(x, 0) &= \Delta_F, & x > x_3 \end{aligned} \quad (4.5)$$

Because  $x_3$  is the pertinent characteristic length in the problem, we can anticipate that  $\overset{N'}{\mathcal{L}}_E$  and  $\overset{N'}{\mathcal{L}}_F$  depend only on  $\eta$  and not upon  $t$ , that is,

$$\overset{N'}{\mathcal{L}}_E = \overset{N'}{\mathcal{L}}_E(\eta) \quad \text{and} \quad \overset{N'}{\mathcal{L}}_F = \overset{N'}{\mathcal{L}}_F(\eta) \quad (4.6)$$

It then follows that equations (4.2) become ordinary differential equations if  $x_3$  has the form

$$x_3 = A \sqrt{\frac{4t^w}{S_c}} \quad (4.7)$$

where the constant  $A$  remains to be determined.

It is not difficult now to obtain solutions that satisfy (4.3)

and (4.5):

$$\begin{aligned} \tilde{C}_X' &= \Delta_X \left[ 1 - \frac{\operatorname{erfc}(-A\eta)}{\operatorname{erfc}(-A)} \right], & x \leq x_s \\ &= 0, & x \geq x_s \\ \tilde{C}_F' &= \Delta_F \left[ 1 - \frac{\operatorname{erfc}(A\eta)}{\operatorname{erfc}(A)} \right], & x \geq x_s \\ &= 0, & x \leq x_s \end{aligned} \quad (4.8)$$

The value of the parameter  $A$  is determined by means of equation (4.4), which yields

$$\operatorname{erf}(A) = \frac{\psi - 1}{\psi + 1} \quad (4.9)$$

$$\text{where } \psi = \frac{\Delta_X f W_F}{\Delta_F \chi W_X} \quad (4.10)$$

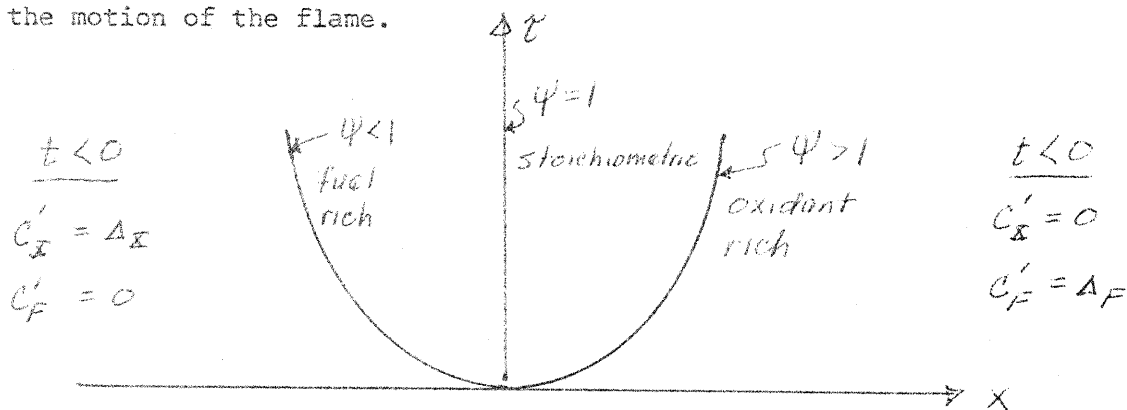
$$\text{and } \operatorname{erf}(A) = \frac{2}{\sqrt{\pi}} \int_0^A e^{-z^2} dz \quad (4.11)$$

$$\operatorname{erfc}(A) = 1 - \operatorname{erf}(A)$$

are the error function and complementary error function.

When  $\psi = 1$ , the value of  $A$  is zero, and the flame remains stationary at  $x = 0$ . When  $\psi > 1$ ,  $A$  is positive and the flame moves into the fuel region. The initial configuration can then be said to be oxidant rich. By moving into the fuel region, the flame produces relative diffusion velocities such

that the flame combustion is always stoichiometric, that is, the flame moves such that the fuel and oxidant are completely annihilated. When  $\psi$  is less than unity,  $A$  is negative and the flame moves into the oxidant region. The initial configuration can then be said to be fuel rich. Correspondingly when  $\psi=1$ , the initial configuration can be said to be stoichiometric. Sketch 2 illustrates the  $X-\xi$  diagram for the motion of the flame.



Sketch 2. Dependence of Flame Motion on  $\psi$ .

Analogous solutions for the flame produced by two streams uniting behind a parabolic cylinder were found by Clarke (1967b), who introduced parabolic coordinates in the study of his steady flow problem. Also some similar conclusions were reached by Clarke and Stegen (1968).

The strength of the flame,  $\tilde{S}'(\xi)$ , can now be determined from (3.28). We obtain

$$\tilde{S}'(\xi) = \frac{\Delta_X}{\lambda W_X} \frac{1}{\sqrt{\pi S'_c \xi}} \frac{e^{-A^2}}{\operatorname{erfc}(-A)} \quad (4.12)$$

The strength of the flame decreases with time and depends of the initial fuel-oxidant ratio.

#### 4.3 Analysis of Flow Field for Stoichiometric Conditions, $\psi = 1$ .

We now consider the flow field when  $\psi = 1$ . In this case the flame is stationary at  $x_s = 0$ . Analogously to Rasmussen and Lake (1973), we use Laplace transforms to analyze the linear initial value problem. We first note from equation (3.20) that

$$\begin{aligned} \phi_p(x, 0) &= -\Delta p / \gamma, & x < 0 \\ &= 0, & x > 0 \end{aligned} \quad (4.13)$$

It can be shown that the higher time derivatives of  $\phi$  vanish at  $t = 0$ . Denoting the Laplace transform of  $\phi(x, t)$  with time as  $\bar{\phi}(x, s)$ , we take the Laplace transform of equation (3.25) and obtain

$$\begin{aligned} (\gamma s + 1) \bar{\phi}_{xxxx} - [(\gamma + P_r) s^2 + P_r s] \bar{\phi}_{xx} + P_r s^3 \bar{\phi} &= \\ -d_F \Delta_F (D_c' - P_r) s e^{-\sqrt{D_c' s} x}, & x > 0 \\ & \\ = -d_X \Delta_X (D_c' - P_r) s e^{+\sqrt{D_c' s} x} & \\ - \frac{P_r s \Delta p}{\gamma}, & x < 0 \end{aligned} \quad (4.14)$$

The solutions to these equations are

$$\begin{aligned} \bar{\varphi} &= A^+ e^{-\lambda_1 x} + B^+ e^{-\lambda_2 x} - \frac{d_F \Delta_F (\mathcal{S}_c - P_r) e^{-\lambda_0 x}}{s K}, \quad x > 0 \\ &= A^- e^{+\lambda_1 x} + B^- e^{+\lambda_2 x} - \frac{d_X \Delta_X (\mathcal{S}_c - P_r) e^{+\lambda_0 x}}{s K} \\ &\quad - \frac{\Delta p}{\gamma s^2}, \quad x < 0 \end{aligned} \quad (4.15)$$

where  $A^+$ ,  $B^+$ ,  $A^-$ , and  $B^-$  are constants of integration and where

$$K \equiv (\mathcal{S}_c - 1)(\gamma \mathcal{S}_c - P_r) s + \mathcal{S}_c (\mathcal{S}_c - P_r) \quad (4.16)$$

$$\lambda_0 \equiv \sqrt{\mathcal{S}_c s} \quad (4.17)$$

$$\lambda_1 \equiv \left[ \frac{(\gamma + P_r) s^2 + P_r s + s \sqrt{[(\gamma - P_r) s + P_r]^2 + 4(P_r - 1) P_r s}}{2(1 + \gamma s)} \right]^{1/2} \quad (4.18)$$

$$\lambda_2 \equiv \left[ \frac{(\gamma + P_r) s^2 + P_r s - s \sqrt{[(\gamma - P_r) s + P_r]^2 + 4(P_r - 1) P_r s}}{2(1 + \gamma s)} \right]^{1/2} \quad (4.19)$$

The transform of the velocity is determined by  $\bar{u}' = \bar{\varphi}_x$ , and the transforms of the density, pressure, and temperature are determined in terms of the potential by means of equations (3.21), (3.20), and (3.16). We have

$$\bar{u}' = -\lambda_1 A^+ e^{-\lambda_1 x} - \lambda_2 B^+ e^{-\lambda_2 x} + \frac{\lambda_0 d_F \Delta_F (\mathcal{S}_c - P_r) e^{-\lambda_0 x}}{s K}, \quad x > 0 \quad (4.20)$$

$$= \lambda_1 A^- e^{+\lambda_1 x} + \lambda_2 B^- e^{+\lambda_2 x} - \frac{\lambda_0 d_X \Delta_X (\mathcal{S}_c - P_r) e^{+\lambda_0 x}}{s K}, \quad x < 0$$

$$\begin{aligned}
 &= -\frac{\alpha_F \Delta_F}{s} - \frac{\lambda_1^2}{s} A^+ e^{-\lambda_1 x} - \frac{\lambda_2^2}{s} B^+ e^{-\lambda_2 x} + \frac{\lambda_0^2 \alpha_F \Delta_F (\delta_C - P_r) e^{-\lambda_0 x}}{s^2 K}, \quad x \geq 0 \\
 &= \frac{\Delta_F}{s} - \frac{\lambda_1^2}{s} A^- e^{\lambda_1 x} - \frac{\lambda_2^2}{s} B^- e^{\lambda_2 x} + \frac{\lambda_0^2 \alpha_I \Delta_I (\delta_C - P_r) e^{\lambda_0 x}}{s^2 K} \quad (4.21), \quad x \leq 0
 \end{aligned}$$

$$\begin{aligned}
 &= \gamma(\lambda_1^2 - s) A^+ e^{-\lambda_1 x} + \gamma(\lambda_2^2 - s) B^+ e^{-\lambda_2 x} \\
 &\quad - \frac{\gamma(\lambda_0^2 - s) \alpha_F \Delta_F (\delta_C - P_r) e^{-\lambda_0 x}}{s K}, \quad x \geq 0 \\
 &= \frac{\Delta_F}{s} + \gamma(\lambda_1^2 - s) A^- e^{\lambda_1 x} + \gamma(\lambda_2^2 - s) B^- e^{\lambda_2 x} \\
 &\quad - \frac{\gamma(\lambda_0^2 - s) \alpha_I \Delta_I (\delta_C - P_r) e^{\lambda_0 x}}{s K}, \quad x \leq 0
 \end{aligned} \quad (4.22)$$

$$\frac{A^+}{s} [\lambda_1^2 (1 + \gamma s) - \gamma s^2] e^{-\lambda_1 x} + \frac{B^+}{s} [\lambda_2^2 (1 + \gamma s) - \gamma s^2] e^{-\lambda_2 x} + \frac{\alpha_F \Delta_F}{s} \left[ 1 - \frac{(\delta_C - P_r)}{s K} \{ \lambda_0^2 (1 + \gamma s) - \gamma s^2 \} \right] e^{-\lambda_0 x} \quad x \geq 0$$

$$\frac{\Delta_I}{s} + \frac{A^-}{s} [\lambda_1^2 (1 + \gamma s) - \gamma s^2] e^{\lambda_1 x} + \frac{B^-}{s} [\lambda_2^2 (1 + \gamma s) - \gamma s^2] e^{\lambda_2 x} + \frac{\alpha_I \Delta_I}{s} \left[ 1 - \frac{(\delta_C - P_r)}{s K} \{ \lambda_0^2 (1 + \gamma s) - \gamma s^2 \} \right] e^{\lambda_0 x} \quad x \leq 0$$

The constants  $A^+$ ,  $B^+$ ,  $A^-$ , and  $B^-$  must now be determined by the continuity and boundary conditions at the flame surface,  $x_3 = 0$ .

#### 4.4 Determination of the Constants $A^+$ , $B^+$ , $A^-$ , $B^-$

At the flame discontinuity,  $x=0$ , the variables  $\bar{u}'$ ,

$\bar{p}'$ ,  $\bar{p}'$ , and  $\bar{T}'$  must be continuous. Since the concentrations  $\bar{c}'_X$  and  $\bar{c}'_F$  are continuous at  $x=0$ , only two variables out of  $\bar{p}'$ ,  $\bar{p}'$ , and  $\bar{T}'$  must be specified continuous and

it follows that the third is from the equation of state (3.16).

A fourth condition to be imposed at  $X=0$  is the temperature jump condition (3.30). With the flame strength determined by (4.12), the Laplace transform of (3.30) leads to

$$\frac{\partial \bar{T}'}{\partial X}(0^+, s) + \frac{P_r \Delta T Q}{S_c \lambda W_{\Sigma}} \frac{\lambda_0}{s} = \frac{\partial \bar{T}'}{\partial X}(0^-, s) \quad (4.24)$$

Imposition of continuity on  $\bar{u}'$ ,  $\bar{p}'$ , and  $\bar{f}'$ , and the jump condition (4.24) at  $X=0$  gives four equations for the constants  $A^+$ ,  $B^+$ ,  $A^-$ , and  $B^-$ . Solving for them yields

$$A^+ = \frac{1}{2(\lambda_1^2 - \lambda_2^2)} \left[ (d_F \Delta F + \Delta p) \frac{(\lambda_2^2 - s)}{s} + \frac{\Delta p}{\gamma} \frac{\lambda_2^2}{s^2} + \frac{E \lambda_0}{\lambda_1(1+\gamma s)} + F(\lambda_1)(\lambda_0^2 - \lambda_2^2) \right] \quad (4.25)$$

$$+ \frac{E \lambda_0}{\lambda_1(1+\gamma s)} + F(\lambda_1)(\lambda_0^2 - \lambda_2^2) \quad (4.26)$$

$$A^- = \frac{-1}{2(\lambda_1^2 - \lambda_2^2)} \left[ (d_F \Delta F + \Delta p) \frac{(\lambda_2^2 - s)}{s} + \frac{\Delta p}{\gamma} \frac{\lambda_2^2}{s^2} - \frac{E \lambda_0}{\lambda_1(1+\gamma s)} - G(\lambda_1)(\lambda_0^2 - \lambda_2^2) \right] \quad (4.27)$$

$$B^+ = \frac{-1}{2(\lambda_1^2 - \lambda_2^2)} \left[ (d_F \Delta F + \Delta p) \frac{(\lambda_1^2 - s)}{s} + \frac{\Delta p}{\gamma} \frac{\lambda_1^2}{s^2} + \frac{E \lambda_0}{\lambda_2(1+\gamma s)} + F(\lambda_2)(\lambda_0^2 - \lambda_1^2) \right] \quad (4.28)$$

$$B^- = \frac{1}{2(\lambda_1^2 - \lambda_2^2)} \left[ (d_F \Delta F + \Delta p) \frac{(\lambda_1^2 - s)}{s} + \frac{\Delta p}{\gamma} \frac{\lambda_1^2}{s^2} - \frac{E \lambda_0}{\lambda_2(1+\gamma s)} - G(\lambda_2)(\lambda_0^2 - \lambda_1^2) \right]$$



where 
$$E \equiv \frac{P_r A_x Q}{S_c \alpha W_x} - (\alpha_x \Delta_x + \alpha_F \Delta_F)$$

$$F(\lambda) \equiv \frac{S_c - P_r}{SK} \left[ (\alpha_x \Delta_x + \alpha_F \Delta_F) \frac{\lambda_0}{\lambda} + (\alpha_F \Delta_F - \alpha_x \Delta_x) \right] \quad (4.29)$$

$$G(\lambda) \equiv \frac{S_c - P_r}{SK} \left[ (\alpha_x \Delta_x + \alpha_F \Delta_F) \frac{\lambda_0}{\lambda} - (\alpha_F \Delta_F - \alpha_x \Delta_x) \right]$$

The solution for the transformed problem is now complete.

We must now concern ourselves with the inversions of these transforms.

In general this must be done approximately, but there is at least one special exact solution of interest.

#### 4.5 Some General Comments.

The Laplace - transformed variables take simplified forms when some of the parameters take particular values. The functions  $F(\lambda)$  and  $G(\lambda)$  vanish when the Lewis number is unity,  $S_c = P_r$ , which is not an unreasonable approximation. When  $P_r = 1$ , the parameters  $\lambda_1$  and  $\lambda_2$ , defined by (4.18) and (4.19), take the simplified values

$$\begin{aligned} \lambda_1 &= \sqrt{5} \\ \lambda_2 &= \frac{5}{\sqrt{1+85}} \end{aligned} \quad (4.30)$$

Here we should recall that the Prandtl number,  $P_r$ , is defined in terms of the reduced viscosity  $\mu_0 \equiv 2\mu_0 + \lambda_0$ . If the Stokes approximation is made,  $\lambda_0 = -\frac{2}{3} \mu_0$ , the value  $P_r = 1$  corresponds to an actual Prandtl number of  $\frac{3}{4}$ , that is,  $\mu_0 c_{p0} / k_0 = \frac{3}{4}$ . This is in accord with many gases, such as air.

We can obtain an approximation for small time by expanding the transforms for large  $s$  and then inverting. As Bienkowski (1965) and Rasmussen and Lake (1973) point out, however, the Navier-Stokes equations may not be valid in this limit, and hence this limiting approximation is not particularly useful, although it may be of some theoretical interest. As the analysis of Rasmussen and Lake illustrates, the limit of  $S \rightarrow 0$  is actually the regime of interest. In this limit,  $\exp(\pm \lambda_2 X)$  plays an essential role that leads to wave behaviour. When the parameters are evaluated in such a way that  $\exp(\pm \lambda_2 X)$  disappears from the problem, then the flow behaviour is entirely diffusive and there is no development of wave motion. We shall demonstrate this by a special exact solution.

It may be possible to obtain exact solutions for special cases somewhat akin to the approach used by Morrison (1956), who utilized certain integral theorems in Laplace transform theory (see Carslaw and Jaeger 1963, pg. 259). These exact solutions are still in fairly complicated forms and not particularly useful for extracting numerical results or physical interpretation. Consequently, we shall use asymptotic-approximation

methods to extract various results of interest.

#### 4.6 A Special Exact Solution.

A wave behaviour in the problem will not appear if the various parameters are evaluated so that  $\exp(\pm \lambda_2 x)$  disappears from the problem. This occurs when the parameters  $B^+$  and  $B^-$  vanish. Perusing (4.27), (4.28), (4.29), and (4.30), we find that  $B^+$  and  $B^-$  vanish when  $P_r = 1$ ,  $\Delta_p = 0$ ,  $E = 0$ , and  $S'_c = P_r$ . It follows from (4.22) that  $\rho' = 0$ , and hence this is a constant-pressure solution. Further, since we have already required that  $\Delta_x f W_F = \Delta_F X W_X$ , the requirement that  $E = 0$  means that the heat-of-reaction,  $Q$ , must have the value

$$Q = X W_X d_X + f W_F d_F \quad (4.31)$$

Perusing the definitions of  $Q$ ,  $d_X$ , and  $d_F$ , we can deduce that (4.31) will be satisfied, at least, if the oxidant, fuel, and product gases are calorically perfect and all have the same ratios of specific heats at the ambient temperature  $T_0$ .

We now find that

$$A^+ = -A^- = - \frac{d_F \Delta_F + \Delta_p}{S} \quad (4.32)$$

With these simple forms we can invert the Laplace transforms by means of standard tables. We obtain

$$u' = (\rho_F \Delta_F + \Delta_f) \frac{e^{-x^2/4\tau}}{\sqrt{\pi\tau}} \quad -\infty < x < \infty \quad (4.33)$$

$$p' = -\rho_F \Delta_F + \frac{1}{2} (\rho_F \Delta_F + \Delta_f) \operatorname{erfc}\left(\frac{x}{2\sqrt{\tau}}\right), \quad -\infty < x < \infty \quad (4.34)$$

$$T' = \frac{1}{2} \left( \Delta_T + \frac{\Delta_x Q}{x W_x} \right) \operatorname{erfc}\left(\frac{x}{2\sqrt{\tau}}\right), \quad x \geq 0 \quad (4.35)$$

$$= \Delta_T + \frac{1}{2} \left( \frac{\Delta_x Q}{x W_x} - \Delta_T \right) \operatorname{erfc}\left(\frac{-x}{2\sqrt{\tau}}\right), \quad x \leq 0$$

The temperature at the flame,  $x=0$ , is

$$T(0, \tau) = \frac{1}{2} \left( \Delta_T + \frac{\Delta_x Q}{x W_x} \right) \quad (4.36)$$

and is a constant. The portion  $\Delta_x Q/x W_x$  is the increase in temperature that arises from the heat of reaction. It is proportional, of course, to the initial amount of oxidant available,  $\Delta_x$ . Notice that the flame does not affect the velocity and density fields, which are continuous in all of their derivatives, except insofar as the initial density discontinuity is specified.

This special problem is a counterpart of the kind of linearized constant-pressure problems discussed by Sforza and Bloom (1965).

4.7 Conditions on the Flame.

The values of the flow variables on the flame,  $X = c'$ , can be evaluated for certain asymptotic situations. The transform of the velocity becomes

$$\begin{aligned} \bar{u}'(0, s) = & \frac{1}{2s(\lambda_1 + \lambda_2)} \left[ \frac{\Delta p}{\delta} \left\{ \frac{\lambda_1, \lambda_2}{s} (1 + \delta s) + \delta s \right\} - \Delta_T \left\{ \lambda_1, \lambda_2 + s \right\} \right. \\ & \left. + (\alpha_F \Delta_F - \alpha_X \Delta_X) \left\{ (\lambda_1, \lambda_2 + s) - \frac{(S_c - P_r)}{K} (\lambda_0 - \lambda_1)(\lambda_0 - \lambda_2) \right\} \right] \end{aligned} \quad (4.37)$$

The transform of the density reduces to

$$\begin{aligned} \bar{\rho}'(0, s) = & \frac{\Delta p - \alpha_F \Delta_F}{2s} - \frac{\lambda_0}{2s(\lambda_1 + \lambda_2)} \left[ \frac{E}{1 + \delta s} \right. \\ & \left. + \frac{(S_c - P_r)}{sK} (\alpha_X \Delta_X + \alpha_F \Delta_F) \left\{ \lambda_0 (\lambda_0 - \lambda_1 - \lambda_2) + \lambda_1, \lambda_2 \right\} \right] \end{aligned} \quad (4.38)$$

The transform of the pressure reduces to

$$\begin{aligned} \bar{p}'(0, s) = & \frac{\Delta p}{2s} + \frac{\delta}{2(\lambda_1 + \lambda_2)} \left[ \frac{E \lambda_0}{1 + \delta s} \left( 1 + \frac{s}{\lambda_1, \lambda_2} \right) \right. \\ & + \frac{S_c - P_r}{sK} (\alpha_X \Delta_X + \alpha_F \Delta_F) \left\{ \lambda_0^2 (\lambda_0 - \lambda_1 - \lambda_2) + \lambda_0 \lambda_1, \lambda_2 \right. \\ & \left. \left. + \frac{s}{\lambda_1, \lambda_2} \left[ \lambda_0 (\lambda_0^2 - \lambda_1^2 - \lambda_1, \lambda_2 - \lambda_2^2) + \lambda_1, \lambda_2 (\lambda_1 + \lambda_2) \right] \right\} \right] \end{aligned} \quad (4.39)$$

The temperature on the flame is given by

$$\bar{T}'(0, s) = \bar{p}'(0, s) - \bar{\rho}'(0, s) \quad (4.40)$$

Consider now the values that obtain for large times.

In this limiting case we consider the limit  $S \rightarrow 0$ . We observe that

$$\lambda_0 = \sqrt{S_0 S}, \quad \lambda_1 \sim \sqrt{P_r S} \left[ 1 - \frac{(\gamma-1)(P_r-1)}{2P_r} S + \dots \right] \quad (4.41)$$

$$\lambda_2 \sim S \left( 1 - \frac{S}{4b^2} + \dots \right), \quad \text{where } b^2 = \frac{P_r}{2(\gamma+P_r-1)}$$

when  $S \rightarrow 0$ . In this limit, we find that the velocity transform behaves as

$$\bar{u}'(0, S) \sim \frac{1}{2S} \left[ \frac{\Delta p}{\gamma} + \left( \frac{\gamma_F \Delta_F - \gamma_X \Delta_X}{\sqrt{S_0}} - \frac{\Delta_T}{\sqrt{P_r}} + \frac{(\gamma-1)}{\gamma \sqrt{P_r}} \Delta p \right) \sqrt{S} + O(S) \right] \quad (4.42)$$

Hence  $u'(0, t)$ , for large time, varies as

$$u'(0, t) \sim \frac{\Delta p}{2\gamma} + \frac{1}{2} \left( \frac{\gamma_F \Delta_F - \gamma_X \Delta_X}{\sqrt{S_0}} - \frac{\Delta_T}{\sqrt{P_r}} + \frac{\gamma-1}{\gamma} \frac{\Delta p}{\sqrt{P_r}} \right) \frac{1}{\sqrt{t}} + O(t^{-1}) \quad (4.43)$$

Thus the velocity that arises because of diffusion and thermal effects dies out with time. The velocity that persists is the gas dynamical part that arises out of the initial pressure disturbance.

The transform of density on the flame approaches the value

$$\bar{\rho}'(0, S) \sim \frac{1}{2S} \left[ \Delta p - \gamma_F \Delta_F - \sqrt{\frac{S_0}{P_r}} E - \left( \sqrt{\frac{S_0}{P_r}} - 1 \right) (\gamma_X \Delta_X + \gamma_F \Delta_F) + O(S^{1/2}) \right] \quad (4.44)$$

Hence we obtain, for large time,

$$p'(0, \tau) \sim \frac{1}{2} \left[ \Delta_F - d_F \Delta_F - \sqrt{\frac{S_c}{P_r}} E - \left( \sqrt{\frac{S_c}{P_r}} - 1 \right) (d_X \Delta_X + d_F \Delta_F) \right] + O(\tau^{-1/2}) \quad (4.45)$$

The density does have a component that arises because of diffusion and the heat of reaction.

The transform of the pressure reduces to

$$\bar{p}'(0, s) \sim \frac{\Delta_p}{2s} + \frac{\gamma}{2\sqrt{P_r} s} \left[ \sqrt{\frac{S_c}{P_r}} E + \sqrt{\frac{S_c}{P_r}} \left( 1 - \frac{P_r}{S_c} \right) (d_X \Delta_X + d_F \Delta_F) \right] + \dots \quad (4.46)$$

Inversion yields the large-time asymptotic behaviour

$$p'(0, \tau) \sim \frac{\Delta_p}{2} + \frac{\gamma}{2\sqrt{P_r}} \sqrt{\frac{S_c}{P_r}} \left[ E + \left( 1 - \frac{P_r}{S_c} \right) (d_X \Delta_X + d_F \Delta_F) \right] \frac{1}{\sqrt{\pi \tau}} + O(\tau^{-1}) \quad (4.49)$$

Just as for the velocity, only the effect of the initial pressure disturbance persists for large time, and the effects of diffusion and heat-of-reaction die out with time.

The temperature, from (4.40), behaves as

$$T'(0, \tau) \sim \frac{1}{2} \left[ \Delta_T + \sqrt{\frac{P_r}{S_c}} \frac{\Delta_X Q}{\chi W_X} \right] + O(\tau^{-1/2}) \quad (4.48)$$

The temperature at the flame is composed of a part due to the initial temperature discontinuity and a part arising from the heat of reaction.

4.8 Solution for Large Time.

For large times the appropriate expansion in the Laplace transforms pertains to  $s \rightarrow 0$ , and  $\lambda_1$ , and  $\lambda_2$  behave as shown by (4.41). In this limit the parameters  $A^+$ ,  $A^-$ ,  $B^+$ , and  $B^-$  take the limiting forms

$$A^+ \sim \frac{1}{2P_T s} \left[ \Delta_T - \frac{\gamma-1}{\gamma} \Delta_P + \sqrt{\frac{P_T}{S_c}} \frac{\Delta_X Q}{\chi W_X} + O(s) \right] \quad (4.49)$$

$$A^- \sim \frac{-1}{2P_T s} \left[ \Delta_T - \frac{\gamma-1}{\gamma} \Delta_P - \sqrt{\frac{P_T}{S_c}} \frac{\Delta_X Q}{\chi W_X} + O(s) \right] \quad (4.50)$$

$$B^+ \sim \frac{-1}{2P_T s} \left[ \frac{\Delta_P}{\gamma} \frac{P_T}{s} + \frac{1}{\sqrt{s}} \frac{P_T}{\sqrt{S_c}} \left\{ \frac{\Delta_X Q}{\chi W_X} - (\gamma_X \Delta_X + \gamma_F \Delta_F) \right\} + \left\{ \frac{\Delta_P}{\gamma} + (P_T - 1)(\gamma_F \Delta_F + \Delta_P) \right\} + \dots \right] \quad (4.51)$$

$$B^- \sim \frac{1}{2P_T s} \left[ \frac{\Delta_P}{\gamma} \frac{P_T}{s} - \frac{1}{\sqrt{s}} \frac{P_T}{\sqrt{S_c}} \left\{ \frac{\Delta_X Q}{\chi W_X} - (\gamma_X \Delta_X + \gamma_F \Delta_F) \right\} + \left\{ \frac{\Delta_P}{\gamma} + (P_T - 1)(\gamma_F \Delta_F + \Delta_P) \right\} + \dots \right] \quad (4.52)$$



In order to demonstrate the effects of the flame as well as the gasdynamic effects that are present without a flame, it is necessary to keep three order of  $S$  in  $B^+$  and  $B^-$ , but only the lowest order in  $A^+$  and  $A^-$  since all the effects appear in the same order in these two parameters.

When  $\lambda_1$  is approximated by  $\lambda_1 \approx \sqrt{P_r S}$  for small  $S$ , the Laplace transforms associated with  $A^+$  and  $A^-$  can be easily inverted. In order to invert those transforms associated with  $B^+$  and  $B^-$ , we must deal with an exponential of the form  $\exp(\pm \lambda_2 X)$ . These terms lead to wave behaviour when  $S$  is small, that is, for large time. Here we make use of the method of Rasmussen and Lake (1973), which is outlined in Appendix B. In the exponential term,  $\lambda_2$  is replaced by

$$\lambda_2 \approx 2b \left[ \sqrt{S + b^2} - b \right] \quad (4.56)$$

where

$$b \equiv \sqrt{\frac{P_r}{2(\gamma + P_r - 1)}}$$

Expression (4.56) is valid to second order when  $S \rightarrow 0$ .

#### 4.9 Velocity Field for Large Time.

When the approximations in the previous section and in Appendix B are utilized, we obtain for the velocity

$$u'(x \geq 0, \tau) \sim \frac{-A_0^+ e^{-P_T x^2/4\tau}}{\sqrt{P_T \pi \tau}} + \frac{\alpha_F \Delta_F e^{-S_0 x^2/4\tau}}{\sqrt{S_0 \pi \tau}} + U_I^+ + U_{II}^+ + U_{III}^+ \quad (4.57)$$

$$u'(x \leq 0, \tau) \sim \frac{A_0^- e^{-P_T x^2/4\tau}}{\sqrt{P_T \pi \tau}} - \frac{\alpha_F \Delta_F e^{-S_0 x^2/4\tau}}{\sqrt{S_0 \pi \tau}} + U_I^- - U_{II}^- + U_{III}^- \quad (4.58)$$

where

$$A_0^+ \equiv \frac{1}{2} \left[ \Delta_T - \frac{\gamma-1}{\gamma} \Delta_P + \sqrt{\frac{P_T}{S_0}} \frac{\Delta_X G}{X W_X} \right] \quad (4.59)$$

$$A_0^- \equiv \frac{-1}{2} \left[ \Delta_T - \frac{\gamma-1}{\gamma} \Delta_P - \sqrt{\frac{P_T}{S_0}} \frac{\Delta_X G}{X W_X} \right] \quad (4.60)$$

$$U_I^+ \equiv \frac{\Delta_P}{2\gamma} \left[ \operatorname{erfc} \left\{ \frac{b(x-\tau)}{\sqrt{\tau}} \right\} + e^{4b^2 x} \operatorname{erfc} \left\{ \frac{b(x+\tau)}{\sqrt{\tau}} \right\} \right] \quad (4.61)$$

$$U_{II}^+ \equiv \frac{1}{2\sqrt{S_0}} \left[ \frac{\Delta_X G}{X W_X} - (\gamma_X \Delta_X + \gamma_F \Delta_F) \right] \frac{bx}{\pi} \int_0^\tau \frac{e^{-\frac{b^2(t-x)^2}{t}}}{\sqrt{\tau-t} t^{3/2}} dt \quad (4.62)$$

$$U_{III}^+ \equiv \frac{1}{2 P_T} \left[ \frac{\Delta_P}{\gamma} \left( 1 - \frac{P_T}{4b^2} \right) + (P_T - 1) (\gamma_F \Delta_F + \Delta_P) \right] \frac{bx e^{-\frac{b^2(\tau-x)^2}{\tau}}}{\sqrt{\pi} \tau^{3/2}} \quad (4.63)$$

$$U_I^-(x, \tau) = U_I^+(-x, \tau) \quad (4.64)$$

$$U_{II}^-(x, \tau) = + U_{II}^+(-x, \tau) \quad (4.65)$$

$$U_{III}^-(x, \tau) = U_{III}^+(-x, \tau) \quad (4.66)$$

The first two exponential terms in (4.57) and (4.58) describe the diffusive-type relaxation of the initial disturbance caused by the disappearance of the diaphragm. This disturbance dies out like  $\mathcal{E}^{-1/2}$ , something akin to the special exact solution (4.33). The functions  $\mathcal{U}_I^{\pm}$ ,  $\mathcal{U}_{II}^{\pm}$ , and  $\mathcal{U}_{III}^{\pm}$  are wave-like in behaviour. The functions  $\mathcal{U}_I^{\pm}$  are the dominating of these three terms, and correspond to a compression wave in one direction and an expansion wave in the other, the directions depending on the value of  $\Delta p$ . Since  $\mathcal{U}_I^{\pm}$  are proportional to  $\Delta p$ , they are of gasdynamic origin and are related to those waves studied by Rasmussen and Lake (1973). In Fig. 1,  $\mathcal{U}_I^{\pm}$  is plotted as function of  $x/\mathcal{E}$  for various values of  $\mathcal{E}$ . As  $\mathcal{E} \rightarrow \infty$ , this plot approaches the results of classical inviscid gasdynamics. The center of the wave front is at  $x/\mathcal{E} = 1$ , where the speed of the front is  $u_0$ .

The functions  $\mathcal{U}_{II}^{\pm}$  describe the waves generated by the flame, which are a pair of compression waves traveling in opposite directions when  $\Delta_I Q / \chi W_X > (\alpha_I \Delta_I + d_F \Delta_F)$  and expansion waves when  $\Delta_I Q / \chi W_X < (\alpha_I \Delta_I + d_F \Delta_F)$ . When the initial pressure differential across the diaphragm,  $\Delta p$ , vanishes,  $\mathcal{U}_I^{\pm}$  also vanish, and  $\mathcal{U}_{II}^{\pm}$  become the dominating wave disturbances. Apparently the quadrature in the definition of  $\mathcal{U}_{II}^{\pm}$  cannot be evaluated in terms of known tabulated functions. When  $\mathcal{E}$  approaches infinity, however, one can establish directly from the Laplace transforms that

$$\sqrt{\tau} U_{II}^+ \propto \left(1 - \frac{x}{\tau}\right)^{-1/2}, \quad \frac{x}{\tau} < 1 \quad (4.67)$$

$$= 0, \quad \frac{x}{\tau} > 1$$

A numerical evaluation of  $U_{II}^+$  is shown in Fig. 2. The magnitude of the disturbance is largest near the wave front, at  $x = \tau$ , which travels with the speed  $a_0$ . The magnitude is associated with the strength of the flame that generated the disturbance. Since the flame strength dies out with time, the strongest part of the disturbance is <sup>at</sup> the wave front, which was generated earliest. The wave front is diffused out because of viscosity and heat conduction. For a fixed value of  $x/\tau$ ,  $U_{II}^+$  dies out approximately like  $\tau^{-1/2}$  except near the wave front. Hence for large time and  $\Delta p \neq 0$ ,  $U_{II}^+$  is small compared to  $U_I^+$ , but it is the dominating disturbance when there is no initial pressure differential.

The functions  $U_{III}^+$  and  $U_{III}^-$  constitute a compression wave traveling in one direction and an expansion wave traveling in the other, the directions depending on the value of the parameters in (4.63). The combination  $\sqrt{\tau} U_{III}^+$  is shown in Fig. 3. This disturbance behaves as a pulse, centered at  $x = \tau$ , and traveling with the speed  $a_0$ . At the wave center,  $x = \tau$ , the magnitude of  $U_{III}^+$  dies out like  $\tau^{-1/2}$ ; hence for large time and  $\Delta p \neq 0$ ,  $U_{III}^+$  is small compared to  $U_I^+$  and acts as a higher order contribution. When there is no initial pressure differential, however,  $U_{III}^+$  becomes significant when  $P_r$  varies significantly from unity. When there is no flame and no initial pressure differential, the entire wave disturbance is associated with  $U_{III}^+$  and vanishes only when  $P_r = 1$ .

#### 4.10 Pressure Field for Large Time.

The corresponding approximations for the pressure become

$$\dot{p}(x \geq 0, \tau) = \frac{\gamma}{2\sqrt{\pi\tau}} \frac{x}{\tau} \left[ \frac{(P_r - 1)}{\sqrt{P_r}} A_0^+ e^{-P_r x^2/4\tau} - \frac{(S_c - 1)}{\sqrt{S_c}} \gamma_F \Delta_F e^{-S_c x^2/4\tau} \right] + \gamma U_I^+ + \gamma U_{II}^+ + \gamma B_0 U_{III}^+ \quad (4.68)$$

$$\dot{p}(x \leq 0, \tau) = \Delta_p - \frac{\gamma}{2\sqrt{\pi\tau}} \frac{x}{\tau} \left[ \frac{(P_r - 1)}{\sqrt{P_r}} A_0^- e^{-P_r x^2/4\tau} - \frac{(S_c - 1)}{\sqrt{S_c}} \gamma_F \Delta_F e^{-S_c x^2/4\tau} \right] - \gamma U_I^- + \gamma U_{II}^- - \gamma B_0 U_{III}^- \quad (4.69)$$

where

$$B_0 = \frac{(P_r - 1) \left[ -\frac{\Delta_p}{\gamma} + \gamma_F \Delta_F + \Delta_p \right]}{\frac{\Delta_p}{\gamma} \left( 1 - \frac{P_r}{P_0} \right) + (P_r - 1) (\gamma_F \Delta_F + \Delta_p)} \quad (4.70)$$

The functions associated with the initial pressure differential,  $\gamma U_I^+$  and  $\gamma U_{II}^-$ , dominate the pressure distribution. The other contributions die out at least as fast as  $\tau^{-1/2}$ . The pressure wave generated by the flame is described by the functions  $\gamma U_{II}^+$  and  $\gamma U_{III}^-$ . When  $\Delta_p = 0$  and there is no flame, the residual pressure wave is described by the functions  $\gamma U_{III}^+$  and  $\gamma U_{III}^-$ , and this contribution vanishes when  $P_r = 1$ .

#### 4.11 Temperature Field for Large Time.

The inversions of the Laplace transforms for the temperature yield, for large time,

$$T'(x \geq 0, \tau) = A_0^+ \operatorname{erfc} \left\{ \frac{x\sqrt{P_r}}{2\sqrt{\tau}} \right\} + (\gamma - 1) U_I^+ + (\gamma - 1) U_{II}^+ + (\gamma - 1) B_1 U_{III}^+ \quad (4.71)$$

$$T'(x \leq 0, \tau) = \Delta_T + A_0^- \operatorname{erfc} \left\{ \frac{-x\sqrt{P_r}}{2\sqrt{\tau}} \right\} - (\gamma - 1) U_I^- + (\gamma - 1) U_{II}^- - (\gamma - 1) B_1 U_{III}^- \quad (4.72)$$

where 
$$B_1 \equiv \frac{\frac{\Delta p}{\gamma} (2 - P_r) + (P_r - 1) (\Delta_F d_F + \Delta_F)}{\frac{\Delta p}{\gamma} \left(1 - \frac{P_r}{4b^2}\right) + (P_r - 1) (d_F \Delta_F + \Delta_F)} \quad (4.73)$$

There are higher-order diffusion terms, akin to the first two terms in (4.68) and the second two terms in (4.69), that have been omitted in the temperature expressions. These terms arise out of terms of  $O(\delta)$  in (4.49) and (4.50). They vanish on the flame and are small elsewhere, but they should be retained when  $\Delta p = 0$  and when there is no flame in order to be consistent with the expressions for the pressure and velocity.

The effect on the temperature field of the flame is shown in Fig. 4. The effects of  $U_{II}^I$  and  $U_{III}^I$  are small and die out with time and hence were omitted in the calculations for Fig. 4. For this calculation the initial temperature jump is taken as zero,  $\Delta_T = 0$ . The temperature at  $X = 0$  is thus due entirely to the flame. For this case the heat of reaction was arbitrarily set equal to

$$\frac{1}{2} \sqrt{\frac{P_r}{Sc}} \frac{\Delta_X Q}{X W_X} = \frac{\gamma - 1}{\gamma} \Delta p$$

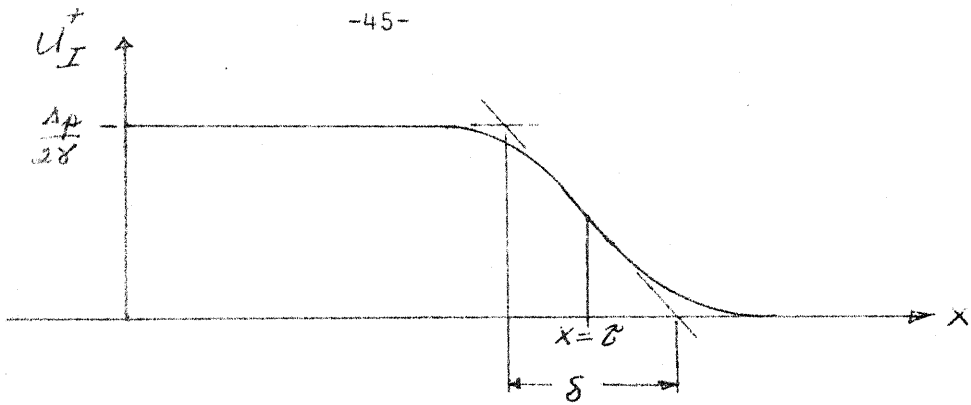
for the purposes of illustration. The corresponding gas dynamic problem with no flame,  $Q = 0$ , is shown in Fig. 5. As for the classical shock-tube problem, the initial pressure difference causes a compression wave to travel to the right and an expansion wave to the left. Without a flame, the contact discontinuity at  $X = 0$  is smoothed out because of thermal conduction. With a flame, the temperature increases at  $X = 0$  because of combustion. The flame is fed by diffusion of oxidant and fuel species, which

tends to cause the temperature to increase with time. This process is balanced off by thermal conduction of energy away from the flame. The fluxes of fuel and oxidant into the flame and of energy away from the flame all decrease with time. The flame temperature adjusts itself to a steady value such that the energy increase because of the heat of reaction is just balanced by the energy decrease caused by thermal conduction.

If there were no initial pressure difference,  $\Delta p = 0$ , then the picture would differ significantly from Fig. 4. The wave fronts would be described primarily by the functions  $U_{II}^+$  and  $U_{II}^-$ , at least when  $P_r \neq 1$  such that  $U_{III}^+$  and  $U_{III}^-$  are negligible. In this case the amplitudes of the wave fronts die out with time, as indicated by Fig. 2. The temperature of the flame, however, would reach a steady-state value as before. The temperature distribution on either side of the flame would be symmetric when  $\Delta T = 0$ ,  $\Delta p = 0$  and  $P_r = 1$ .

#### 4.12 Thickness of Pressure-Induced Wave Front.

In Figs. 1 to 5 the wave fronts appear to be steepening as  $\mathcal{Z} \rightarrow \infty$ . This occurs because the amplitude is plotted as a function of  $X/\mathcal{Z}$  and means that the width of the wave front is becoming smaller compared to the extent of the disturbance, that is, compared to  $\mathcal{Z}$ . When the amplitude is plotted as a function of  $X$ , the width of the wave front is found to increase with  $\mathcal{Z}$ , that is, the wave front tends to flatten out. With the use of sketch 3, we can evaluate the width of the wave front analytically. The wave front associated with the initial pressure differential,  $U_I^+$ , is shown in Sketch 3 at a given instant.



Sketch 3. Wave-Front Thickness.

We define the nondimensional thickness of the wave front as

$$\delta \equiv \frac{\Delta p / 2\gamma}{\left(\frac{\partial U_I^+}{\partial x}\right)_{x=\zeta}} \quad (4.74)$$

Making use of formula (4.61), we obtain, for large  $\zeta$ ,

$$\delta = \frac{\sqrt{\pi}\zeta}{b} = \sqrt{\frac{2\pi(\gamma + P_r - 1)\zeta}{P_r}} \quad (4.75)$$

The thickness of the front increases like the square root of  $\zeta$ .

It also depends on the ratio of specific heats,  $\gamma$ , and the reduced Prandtl number,  $P_r$ , of the ambient gas. The variation of the wave-front thickness with  $P_r$  is shown in Fig. 6. For values of  $P_r$  near unity and greater, the variation in  $\delta$  is small. The dependance on  $\gamma$  is also weak.

The viscosity and heat conduction in the linearized problem cause the wave front to spread. On the other hand, it is well known that the nonlinearities in the problem cause compression waves to steepen and expansion waves to flatten. The balance between the steepening of the nonlinearities and the flattening of the viscosity leads to the formation of shock waves. It transpires that the second-order theory, corresponding to the present linear



theory, breaks down because of both nonlinear and dissipative effects. The breakdown appears in the form of secularities, and the solution is not uniformly valid in the far field. A recent analysis dealing with this behaviour is given by Halabisky and Sirovich (1973).

We can deal with this nonuniform behaviour in this linear analysis by interpreting the nondimensional time,  $\mathcal{L}$ , as a combination of a Reynolds number,  $\rho_0 a_0 L / \mu_0$ , and a wave time,  $\frac{a_0 t}{L}$ , where  $L$  is some characteristic length of interest. We then have

$$\mathcal{L} \equiv \frac{\rho_0 a_0^2 t}{\mu_0} = \frac{\rho_0 a_0 L}{\mu_0} \left( \frac{a_0 t}{L} \right) \quad (4.76)$$

We can now regard the wave time as fixed and of order unity.

The time  $\mathcal{L}$  is then large by virtue of the Reynolds number being large. The far-field non-uniformities, on the other hand, are associated with holding the Reynolds number fixed and letting the wave time grow large.

#### 4.13 Radiation in an Optically Thick Medium.

When the departure from radiation equilibrium is small, a gas can be classified as optically thick (see Vincenti and Kruger 1965). In this case the radiative heat flux can be expressed by the Rosseland diffusion approximation:

$$\vec{q}^R = -k_R \text{grad } T \quad (4.77)$$

where

$$k_R = \frac{16 \sigma T^3}{3 \chi_R}$$

and  $\sigma$  and  $\chi_R$  are the Stefan-Boltzmann constant and the Rosseland mean absorption coefficient. Omitting contributions of diffusion, we can write the total heat flux vector as

$$\vec{q} = - (k + k_R) \text{grad } T \quad (4.78)$$

where  $k$  is the molecular conductivity and  $k_R$  the radiative conductivity.

The effects of radiation in an optically thick medium can easily be incorporated into the present analysis. The reduced Prandtl number can be rewritten as

$$P_r = \frac{\tilde{u}_0 c_{p_0}}{k_0 + k_{R_0}} \quad (4.79)$$

The effect of optically thick radiation is thus to effectively reduce the Prandtl number below its ordinary molecular value.

When  $k_{R_0} \gg k_0$ , the effective Prandtl number becomes small.

#### 4.14 Discontinuities Across the Flame Sheet

We have asserted that the velocity, pressure, density, temperature and concentration are continuous across the flame sheet. In addition, the velocity gradient is continuous across the sheet, as established by (2.17). Further, we have established that the concentration gradients and temperature gradients are discontinuous across the flame sheet and computed the value of the jumps. The density gradient, pressure gradient, and second derivative of the velocity are also discontinuous across the flame

sheet, and we now wish to evaluate the jumps in these quantities for the one-dimensional shock-tube problem.

The jump in the Laplace transform of the density gradient across the flame sheet can be determined from (4.12). We obtain

$$\left[ \frac{\partial \bar{p}'}{\partial x} \right]_0^-^{0^+} = \frac{E}{1+\gamma S} \sqrt{\frac{S c}{S}} \quad (4.80)$$

where  $E$  is given by (4.29). By means of the convolution theorem, the inversion of (4.80) can be written

$$\left[ \frac{\partial p'}{\partial x} \right]_0^-^{0^+} = \frac{E \sqrt{S c}}{\gamma \sqrt{\pi}} \int_0^t \frac{e^{-t/\gamma}}{\sqrt{\gamma^2 - t}} dt \quad (4.81)$$

For large time the asymptotic expansion of (4.81) is

$$\left[ \frac{\partial p'}{\partial x} \right]_0^-^{0^+} \sim \frac{E \sqrt{S c}}{\sqrt{\pi}} \left[ \frac{1}{\gamma^{1/2}} + \frac{\gamma}{2 \gamma^{3/2}} + \dots \right] \quad (4.82)$$

Thus the discontinuity in the density gradient dies out as one over the square root of time.

The Laplace transform of the pressure gradient can be determined from (4.22) or from (3.16) since the density, temperature, and concentration gradients are known. We obtain

$$\left[ \frac{\partial \bar{p}'}{\partial x} \right]_0^-^{0^+} = - \frac{\gamma S E}{1+\gamma S} \sqrt{\frac{S c}{S}} \quad (4.83)$$

From this expression we can deduce that

$$\left[ \frac{\partial p'}{\partial x} \right]_{0^-}^{0^+} = -\gamma \frac{\partial}{\partial \tau} \left[ \frac{\partial p'}{\partial x} \right]_{0^-}^{0^+} \quad (4.84)$$

which could have been deduced directly from (3.20) and (3.21).

Inversion of (4.83) yields

$$\left[ \frac{\partial p'}{\partial x} \right]_{0^-}^{0^+} = \frac{E \sqrt{S_c}}{\sqrt{\pi}} \left[ \frac{1}{\gamma} \int_0^{\tau} \frac{e^{-t/\gamma}}{\sqrt{\tau-t}} dt - \frac{1}{\sqrt{\tau}} \right] \quad (4.85)$$

The asymptotic expansion for large times is

$$\left[ \frac{\partial p'}{\partial x} \right]_{0^-}^{0^+} \sim \frac{E \sqrt{S_c}}{\sqrt{\pi}} \frac{\gamma}{2 \tau^{3/2}} + O(\tau^{-5/2}) \quad (4.86)$$

Thus the discontinuity in the pressure gradient dies out faster than the discontinuities in the other gradients.

The discontinuity in the second derivative of the velocity can be obtained from either of equations (3.20) or (3.21).

We get

$$\left[ \frac{\partial^2 u}{\partial x^2} \right]_{0^-}^{0^+} = \frac{1}{\gamma} \left[ \frac{\partial p'}{\partial x} \right]_{0^-}^{0^+} \quad (4.87)$$

Thus the jump in the second derivative of the velocity dies out like  $\tau^{-3/2}$  for large time, just as for the pressure gradient.

The weaker discontinuities in the velocity and pressure for this problem are akin to the velocity and pressure being continuous across the contact - surface discontinuity in the classical inviscid shock-tube problem whereas the other variables are all discontinuous.

That the density gradient is discontinuous across the flame sheet derives from the fact that the linearized equations were used in the analysis. If the nonlinear equations were utilized, the density gradient would be continuous. This can be seen from the continuity equation, which, when the non-linear terms are written on the right-hand side, appears as

$$\frac{\partial \rho'}{\partial t} + \frac{\partial u'}{\partial x} = -\rho' \frac{\partial u'}{\partial x} - u' \frac{\partial \rho'}{\partial x}$$

Since  $\rho'$  and  $\frac{\partial u'}{\partial x}$  are continuous, it follows that  $\frac{\partial \rho'}{\partial x}$  is continuous. If the linearized equations are used also in the analysis of the structure of the flame, that is, in the "inner" problem (see section 6), the discontinuities are smoothed out by virtue of the matching conditions. This, of course, would also be true for the nonlinear problem, but the nonlinear analysis would be a far more difficult proposition.

## 5. WEAK SPHERICAL EXPLOSION

### 5.1 Description and Initial Conditions

Consider a spherical diaphragm at  $\bar{r} = \bar{r}_0$ . Outside this sphere,  $\bar{r} > \bar{r}_0$ , let there be a mixture of product gas and a small amount of fuel gas. Inside the sphere,  $\bar{r} < \bar{r}_0$ , let there be a mixture of product gas and a small amount of oxidant gas. Let the temperature and pressure inside the sphere differ by small amounts from the prevailing ambient conditions outside the sphere. At the instant  $\bar{t} = 0$ , the diaphragm instantly disappears, and we wish to determine the subsequent development of the flow field.

We assume that the ambient temperature and density,  $T_0$  and  $\rho_0$ , are sufficiently high that combustion is immediately initiated.

The initial conditions are depicted in Sketch 4.

$\bar{r} < \bar{r}_0, t < 0$

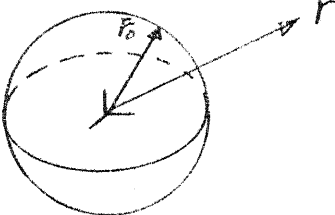
$\rho' = \Delta\rho$

$\rho' = \Delta\rho$

$T' = \Delta T$

$C'_X = \Delta X$

$C'_F = 0$



$\Delta\rho = \Delta\rho + \Delta T + d_X \Delta X$

$\bar{r} > \bar{r}_0, t < 0$

$\rho' = 0$

$\rho' = -d_F \Delta F$

$T' = 0$

$C'_X = 0$

$C'_F = \Delta F$

Sketch 4. Initial Conditions and Configuration for the Sphere.

Again we introduce nondimensional variables as described in Section

3. The flame is at the position  $\bar{r} = \bar{r}_s(t)$ , where  $\bar{r}_s(0) = \bar{r}_0$ .

5.2 The Problem for the Concentrations and Flame Position

The diffusion equations in spherical coordinates are

$$S_c \frac{\partial C'_X}{\partial \bar{t}} = \frac{\partial^2 C'_X}{\partial \bar{r}^2} + \frac{2}{\bar{r}} \frac{\partial C'_X}{\partial \bar{r}}, \quad \bar{r} < \bar{r}_s \quad (5.1)$$

$$S_c \frac{\partial C'_F}{\partial \bar{t}} = \frac{\partial^2 C'_F}{\partial \bar{r}^2} + \frac{2}{\bar{r}} \frac{\partial C'_F}{\partial \bar{r}}, \quad \bar{r} > \bar{r}_s \quad (5.2)$$

The initial conditions are

$$C'_X(\bar{r}, 0) = \Delta X, \quad \bar{r} < \bar{r}_0 \quad (5.3)$$

$$C'_F(\bar{r}, 0) = \Delta F, \quad \bar{r} > \bar{r}_0$$

The boundary conditions at the origin and infinity are

$$\begin{aligned} \frac{\partial C'_X}{\partial r}(0, \tau) &= 0 \\ \frac{\partial C'_F}{\partial r}(\infty, \tau) &= 0 \end{aligned} \tag{5.4}$$

The boundary conditions at the flame are

$$\begin{aligned} C'_X(r_s(\tau), \tau) &= 0 \\ C'_F(r_s(\tau), \tau) &= 0 \end{aligned} \tag{5.5}$$

$$\frac{\partial C'_X}{\partial r}(r_s, \tau) = -\frac{\Delta_X}{\Delta_F} \psi^{-1} \frac{\partial C'_F}{\partial r}(r_s, \tau), \tag{5.6}$$

where

$$\psi \equiv \frac{\Delta_X f W_F}{\Delta_F X W_X} \tag{5.7}$$

### 5.3 Approximation for Large Reynolds Numbers and Corresponding Small Time

For suitably short times the flame will not travel far from its original position at the diaphragm  $\bar{r} = \bar{r}_0$ . When  $\bar{r}_0$  is appropriately large, the flow will appear to be one dimensional. The pertinent nondimensional variables (unbarred space variables) are defined by (3.3). We now wish to establish an approximation that is valid when the time  $\tau$  is fixed and the Reynolds number  $r_0$  is suitably large, or when  $r_0$  is fixed and  $\tau$  is suitably small. We begin by transferring the origin to the position of the diaphragm by means of the transformation

$$\begin{aligned} z &= r - r_0 \\ z_s(r) &= r_s(r) - r_0 \end{aligned} \tag{5.8}$$

We also treat the Reynolds number  $r_0$  as large and introduce a small parameter  $\epsilon$  defined as

$$\epsilon \equiv \frac{1}{r_0} \tag{5.9}$$

In terms of the new variables the diffusion equations become

$$Sc \frac{\partial c'_I}{\partial \tau} = \frac{\partial^2 c'_I}{\partial z^2} + \frac{2\epsilon}{1+\epsilon z} \frac{\partial c'_I}{\partial z} \tag{5.10}$$

$$Sc \frac{\partial c'_F}{\partial \tau} = \frac{\partial^2 c'_F}{\partial z^2} + \frac{2\epsilon}{1+\epsilon z} \frac{\partial c'_F}{\partial z}$$

The initial and boundary conditions become

$$\left. \begin{aligned} c'_I(z, 0) &= \Delta_I, & z < 0 \\ c'_F(z, 0) &= \Delta_F, & z > 0 \end{aligned} \right\} \tag{5.11}$$

$$\left. \begin{aligned} \frac{\partial c'_I}{\partial z} \left( -\frac{1}{\epsilon}, \tau \right) &= 0 \\ \frac{\partial c'_F}{\partial z} \left( \infty, \tau \right) &= 0 \end{aligned} \right\} \tag{5.12}$$



$$\left. \begin{aligned} c'_X(z_s, \tau) &= 0 \\ c'_F(z_s, \tau) &= 0 \end{aligned} \right\} \quad (5.13)$$

$$\frac{\partial c'_X}{\partial z}(z_s, \tau) = - \frac{\Delta_X}{\Delta_F} \psi^{-1} \frac{\partial c'_F}{\partial z}(z_s, \tau) \quad (5.14)$$

We develop an asymptotic approximation for small  $\epsilon$  by means of the following expansions:

$$c'_X \sim c_{X_0} + \epsilon c_{X_1} + \epsilon^2 c_{X_2} + \dots \quad (5.15)$$

$$c'_F \sim c_{F_0} + \epsilon c_{F_1} + \epsilon^2 c_{F_2} + \dots \quad (5.16)$$

$$z_s(\tau) = f_0(\tau) + \epsilon f_1(\tau) + \epsilon^2 f_2(\tau) + \dots \quad (5.17)$$

These expansions are to be substituted into the diffusion equations, initial and boundary conditions, and terms of corresponding powers of  $\epsilon$  collected. Since  $\epsilon$  is small but arbitrary, the collected coefficients of each powers of  $\epsilon$  must vanish. In this way a hierarchy of equations and auxiliary conditions for each order of approximation is established. We should note that the boundary conditions (5.13) and (5.14) involve a transfer of the flame conditions to the unknown zeroth-order position of the flame. This is done by means of a Taylor expansion of the form

$$\Phi(z_s, t) = \Phi(f_0, t) + \epsilon f_1 \frac{\partial \Phi}{\partial z}(f_0, t) + O(\epsilon^2) \quad (5.18)$$

The equations for the zeroth-order problem are exactly the same as for the one-dimensional shock-tube problem which was solved in Section 4.1. The solutions for  $C_{X_0}$  and  $C_{F_0}$  are given by (4.8), and  $f_0(t)$  is given by (4.7) and (4.9). The equations and auxiliary conditions for the first-order problem are

$$\begin{aligned} S_c \frac{\partial C_{X_1}}{\partial t} - \frac{\partial^2 C_{X_1}}{\partial z^2} &= 2 \frac{\partial C_{X_0}}{\partial z}, & z < z_s \\ S_c \frac{\partial C_{F_1}}{\partial t} - \frac{\partial^2 C_{F_1}}{\partial z^2} &= 2 \frac{\partial C_{F_0}}{\partial z}, & z > z_s \end{aligned} \quad (5.19)$$

$$\left. \begin{aligned} C_{X_1}(z, 0) &= 0 \\ C_{F_1}(z, 0) &= 0 \end{aligned} \right\} \quad (5.20)$$

$$\left. \begin{aligned} \frac{\partial C_{X_1}}{\partial z}(-\infty, t) &= 0 \\ \frac{\partial C_{F_1}}{\partial z}(\infty, t) &= 0 \end{aligned} \right\} \quad (5.21)$$

$$\left. \begin{aligned} C_{X_1}(f_0, t) + f_1(t) \frac{\partial C_{X_0}}{\partial z}(f_0, t) &= 0 \\ C_{F_1}(f_0, t) + f_1(t) \frac{\partial C_{F_0}}{\partial z}(f_0, t) &= 0 \end{aligned} \right\} \quad (5.22a)$$

$$\frac{\partial C_{I1}}{\partial z}(f_0, \tau) + f_1(\tau) \frac{\partial^2 C_{I0}}{\partial z^2}(f_0, \tau) =$$

$$-\frac{\Delta_I}{\Delta_F} \psi^{-1} \left[ \frac{\partial C_{F1}}{\partial z}(f_0, \tau) + f_1(\tau) \frac{\partial^2 C_{F0}}{\partial z^2}(f_0, \tau) \right] \quad (5.23a)$$

We note from the zeroth-order solution (4.8) that

$$\frac{\partial C_{I0}}{\partial z} = -\frac{\Delta_I}{\operatorname{erfc}(-A)} \frac{1}{\sqrt{\pi}} \frac{A}{f_0} e^{-A^2 z^2 / f_0^2}$$

$$\frac{\partial C_{F0}}{\partial z} = \frac{\Delta_F}{\operatorname{erfc}(A)} \frac{1}{\sqrt{\pi}} \frac{A}{f_0} e^{-A^2 z^2 / f_0^2}$$

$$\frac{\partial^2 C_{I0}}{\partial z^2} = -\frac{2A^2 z}{f_0^2} \frac{\partial C_{I0}}{\partial z}$$

$$\frac{\partial^2 C_{F0}}{\partial z^2} = -\frac{2A^2 z}{f_0^2} \frac{\partial C_{F0}}{\partial z}$$

With these results, (5.22) and (5.23) become

$$\left. \begin{aligned} C_{X_1}(f_0, \tau) &= \frac{\Delta_X}{\operatorname{erfc}(-A)} \frac{\partial A}{\partial \tau} \frac{f_1}{f_0} e^{-A^2} \\ C_{F_1}(f_0, \tau) &= - \frac{\Delta_F}{\operatorname{erfc}(A)} \frac{\partial A}{\partial \tau} \frac{f_1}{f_0} e^{-A^2} \end{aligned} \right\} \quad (5.22b)$$

$$\frac{\partial C_{X_1}}{\partial z}(f_0, \tau) = - \frac{\Delta_X}{\Delta_F} \psi^{-1} \frac{\partial C_{F_1}}{\partial z}(f_0, \tau) \quad (5.23b)$$

By Laplace transforms or other means, one may establish that the solution to this problem is

$$C_{X_1}(z, \tau) = - \frac{\Delta_X}{\operatorname{erfc}(-A)} \frac{f_0}{A\sqrt{\pi}} e^{-A^2 z^2 / f_0^2} \quad (5.24)$$

$$C_{F_1}(z, \tau) = \frac{\Delta_F}{\operatorname{erfc}(A)} \frac{f_0}{A\sqrt{\pi}} e^{-A^2 z^2 / f_0^2} \quad (5.25)$$

$$f_1(\tau) = - \frac{f_0^2}{2A^2} \quad (5.26)$$

where, from (4.7),  $f_0$  is given by

$$f_0(\tau) = A \sqrt{\frac{4\tau}{S_c}} \quad (5.27)$$

and  $A$  is determined in terms of  $\psi'$  by (4.9).

If the flame is to remain close to its origin, and if the first order correction is to be small, then  $A$  and  $\zeta$  must be restricted by

$$\epsilon / f_0 + \epsilon f_1 \ll 1 \quad (5.28)$$

If  $A$  and  $S_c'$  are of order unity, then we can express the limitation as

$$\epsilon \zeta^{1/2} \ll 1$$

or 
$$\zeta \ll \frac{1}{\epsilon^2} \quad (5.29)$$

Writing  $\zeta$  in terms of the wave time,  $\tau_w \equiv a_0 t / \bar{r}_0$ , such that

$$\zeta = \tau_0 \tau_w \quad (5.30)$$

and recalling that  $\epsilon \equiv \tau_0^{-1}$ , we can recast the restriction (5.29) in terms of the wave time as

$$\tau_w \ll \tau_0 \quad (5.31)$$

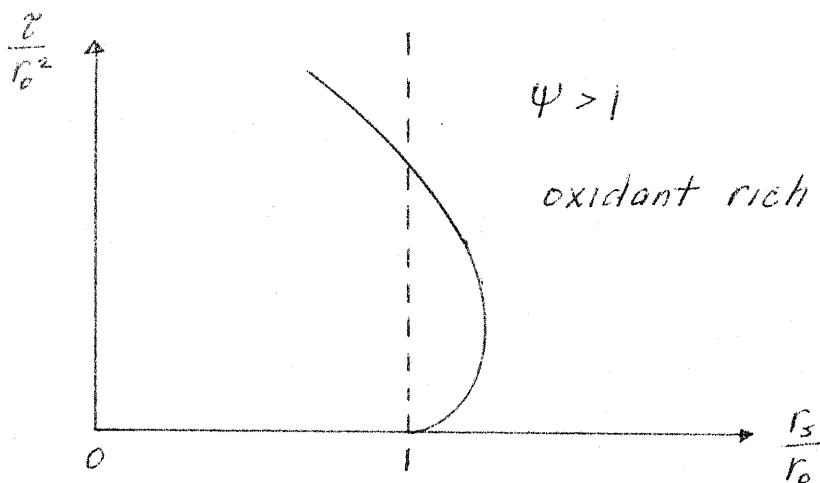
Thus for wave times of order unity and large Reynolds numbers,  $\tau_0$ , the above perturbation solution will be valid, and the wave processes will transpire before the flame moves significantly from its original position.

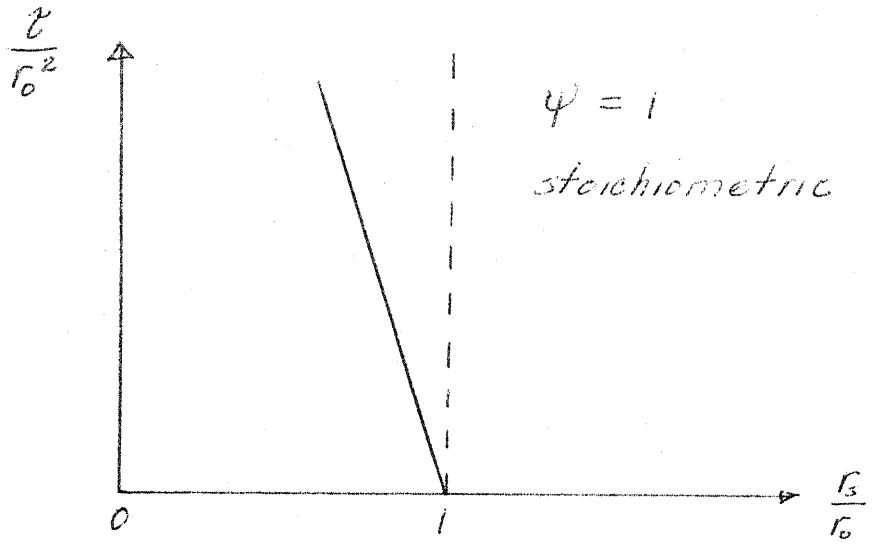
### 5.4 Position of the Spherical Flame

The flame position, subject to (5.29), can be written as

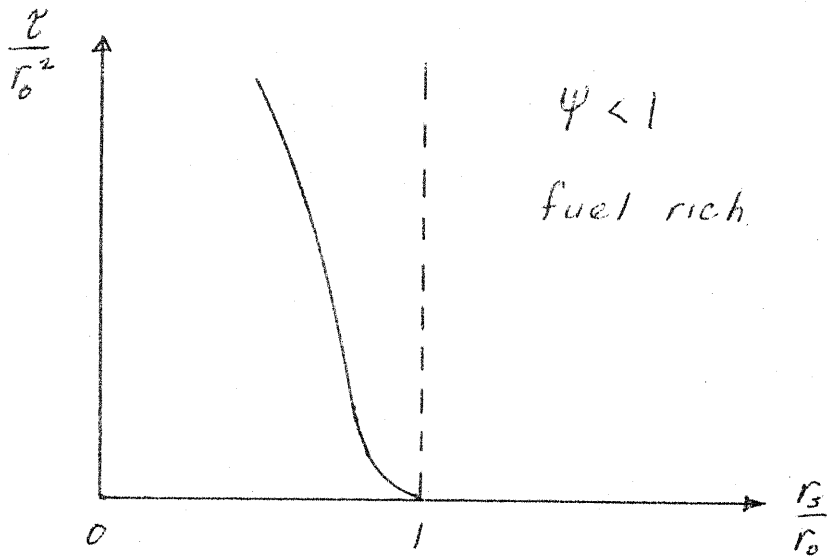
$$\frac{r_s(\tau)}{r_0} = 1 + A \sqrt{\frac{4\tau}{Sc r_0^2}} - \frac{2\tau}{Sc r_0^2} + O\left(\frac{\tau^{3/2}}{r_0^3}\right) \quad (5.32)$$

The third term on the right-hand side, which arises from the spherical geometry, always causes the flame to travel towards the center of the sphere. The second term may be either positive or negative, depending on the value of  $A$ . When  $A$  is positive, that is, when  $\psi'$  is greater than unity corresponding to the initial conditions being oxidant rich, the flame travels outward initially and then travels inward. This is shown in Sketch 5a.





(b)



(c)

Sketch 5. Position of the Spherical Flame

When stoichiometric initial conditions prevail ( $\psi = 1, A = 0$ ), the flame travels inwardly linearly with time, as shown in Sketch 5b. When the initial conditions are fuel rich,  $\psi < 1$ , the flame travels inward very rapidly at the beginning and then approaches the linear behaviour with time, as shown in Sketch 5c. Because the species outside the sphere is of infinite extent and the species inside the sphere is of finite extent, the species inside the sphere tends to be used up. Consequently, the flame will ultimately travel inward in order to add a relative diffusion rate of the vanishing inside species and thus maintain stoichiometric combustion relative to the flame. When the flame reaches the origin one species has been completely consumed and the flame becomes extinguished. The approximations derived here are not valid near this limit, of course.

### 5.5 Flame Strength and Temperature-Gradient Jump

With the concentration fields now determined the flame strength,  $\tilde{S}^*$ , and temperature-gradient jump can be determined from equations (3.28) and (3.30). For the flame strength, the terms of order  $\epsilon$  cancel out, and we obtain

$$\tilde{S}^*(r) = \frac{A_{\epsilon}}{x W_{\epsilon} \sqrt{\pi} s_{\epsilon} r} \frac{e^{-A^2}}{\operatorname{erfc}(-A)} \left[ 1 + O(\epsilon^2) \right] \quad (5.33)$$

Thus, with terms of order  $\epsilon^2$  omitted, the flame strength is the same as for the one-dimensional problem.



With the flame strength thus determined, the temperature-gradient is determined by (3.30):

$$\left[ \frac{\partial T'}{\partial r} \right]_{r_s^-}^{r_s^+} = -L_r Q \tilde{S}(r)$$

### 5.6 Further Comments

The work on spherical flames presented in section 5 was done in collaboration with *Ms.* Karen Frair, a Ph.D. candidate at the University of Oklahoma. The continuation of the spherical explosion problem, something akin to the one-dimensional shock-tube problem investigated herein, is part of her doctoral dissertation which will be completed in September 1974.

## 6. STRUCTURE OF THE DIFFUSION FLAME

### 6.1 Preliminary Remarks

The preceding analysis that treats the flame as a discontinuity surface imbedded in the flow field is the outer expansion in a scheme of matched asymptotic expansions. The complementary inner expansion of this scheme deals with the structure of the flame itself. Treatment of steady flows with flames by means of inner and outer expansions has been developed previously. Here we make use of the analysis of Clarke (1967b) whose mathematical problem, although one of steady flow, is very similar in nature to ours. References to previous work are given in Clarke's paper. Here we consider only "reaction-broadened" flames for which the reverse reaction time is so long that it can be set equal to infinity and only fast forward reactions considered in the combustion process. Thus we consider reaction described by (2.25) with  $\mathcal{L}_r = \infty$  and  $\mathcal{L}_f$  considered as very small. We restrict ourselves to the one-dimensional shock-tube problem for  $\psi = 1$ .

### 6.2 The Problem for the Species Concentrations

The flame is not actually a discontinuity surface but a region over a small width of the field where the reaction rate is very large by virtue of  $\mathcal{L}_f$  going to zero. We therefore introduce a stretched coordinate by

$$Y = \frac{X}{\epsilon^m}, \quad m > 0 \quad (6.1)$$

where  $E = \tilde{c}_f$  and  $X, \tilde{c}$ , and  $\tilde{c}_f$  are normalized by the viscous parameters as given by (3.3). The exponent  $m$  is to be determined so that the inner solution can be matched with the outer. The species conservation equations (2.2) can be now written

$$E^{2m} S_c' \frac{\partial C_X'}{\partial Y} - \frac{\partial^2 C_X'}{\partial Y^2} = -E^{2m-1} X W_X S_c' C_X^x C_F^f \quad (6.2)$$

$$E^{2m} S_c' \frac{\partial C_F'}{\partial Y} - \frac{\partial^2 C_F'}{\partial Y^2} = -E^{2m-1} F W_F S_c' C_X^x C_F^f$$

We now seek an inner expansion of the form

$$C_X' = E^\eta C_{X1} + E^{2\eta} C_{X2} + \dots \quad (6.3)$$

$$C_F' = E^\eta C_{F1} + E^{2\eta} C_{F2} + \dots$$

where again  $\eta$  must be determined so that matching is possible. The diffusion terms will now balance the forward reaction terms if

$$2m + (-1 + X + F)\eta - 1 = 0 \quad , \quad (6.4)$$

and to lowest order we have

$$\frac{\partial^2 C_{X1}}{\partial Y^2} = X W_X S_c' C_{X1}^x C_{F1}^f \quad (6.5)$$

$$\frac{\partial^2 C_{F1}}{\partial Y^2} = F W_F S_c' C_{X1}^x C_{F1}^f$$

Elimination of  $c_{II}^x$   $c_{FI}^f$  between the last two equations yields

$$\frac{\partial^2 c_{FI}}{\partial Y^2} = \frac{f W_F}{x W_X} \frac{\partial^2 c_{XI}}{\partial Y^2} \quad (6.6)$$

A first integration yields

$$\frac{\partial c_{FI}}{\partial Y} = \frac{f W_F}{x W_X} \frac{\partial c_{XI}}{\partial Y} + a_0(\tau) \quad (6.7)$$

where  $a_0(\tau)$  is a function of integration that depends on time. At this stage we can evaluate  $m$  and  $n$  so that the outer limit of the inner solution matches the inner limit of the outer solution, that is,

$$\begin{aligned} \frac{\partial c_{FI}}{\partial Y}(\infty, \tau) &= \frac{\partial c'_F}{\partial X}(0^+, \tau) \\ \frac{\partial c_{XI}}{\partial Y}(\infty, \tau) &= \frac{\partial c'_X}{\partial X}(0^+, \tau) = 0 \\ \frac{\partial c_{FI}}{\partial Y}(-\infty, \tau) &= \frac{\partial c'_F}{\partial X}(0^-, \tau) = 0 \\ \frac{\partial c_{XI}}{\partial Y}(-\infty, \tau) &= \frac{\partial c'_X}{\partial X}(0^-, \tau) \end{aligned} \quad (6.8)$$

Expressions (6.8) can be written independent of  $\epsilon$  only since  $a_0(\tau)$  is independent of  $\epsilon$ , from which it was deduced that  $m = n$ , and hence from (6.4) that

$$m = n = \frac{1}{1 + x + f} \quad (6.9)$$

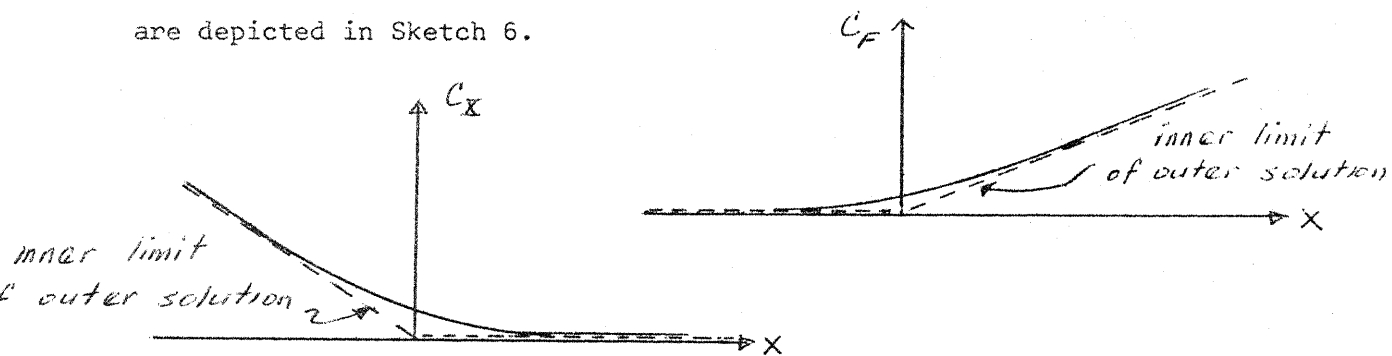
We further deduce that

$$\begin{aligned}
 a_0(\tau) &= \frac{\partial C_F'}{\partial X}(0^+, \tau) \\
 &= \Delta_F \sqrt{\frac{S_C}{\pi \tau}}
 \end{aligned}
 \tag{6.10}$$

This is in accord with (3.29) for  $\psi=1$ . A further integration of (6.7) yields

$$C_{FI} = \frac{\Delta_F}{\Delta_X} C_{II1} + a_0 Y, \tag{6.11}$$

where the new function of integration is found to vanish as a consequence of matching. The inner solutions for the concentrations are depicted in Sketch 6.



Sketch 6. Inner Solution for the Concentrations

A single equation for the concentration  $C_{II1}$  can be obtained by substituting (6.11) into (6.5):

$$\frac{\partial^2 C_{II1}}{\partial Y^2} = X \frac{W_X}{S_C} C_{II1} \left( \frac{\Delta_F}{\Delta_X} C_{II1} + a_0 Y \right)^F \tag{6.12}$$

The boundary conditions are

$$C_{\mathcal{E}1} = 0, \quad Y = \infty$$

$$C_{\mathcal{E}1} \sim a_0 \frac{\Delta_{\mathcal{E}}}{\Delta_F} Y, \quad Y \rightarrow \infty$$

(6.13)

The governing equation (6.12) and boundary conditions (6.13) can be put in a simpler, symmetric form by means of the transformation

$$C_{\mathcal{E}1} = \alpha \mathcal{L}(z) - \frac{a_0(z)}{2} \frac{\Delta_{\mathcal{E}}}{\Delta_F} Y$$

$$Y = \beta(z) z$$

(6.14)

where

$$\alpha(z) \equiv \left[ \left( \frac{a_0(z)}{2} \frac{\Delta_{\mathcal{E}}}{\Delta_F} \right)^2 \left( \frac{\Delta_{\mathcal{E}}}{\Delta_F} \right)^f \frac{1}{x W_x S_c} \right]^m$$

$$\beta(z) \equiv \frac{2}{a_0(z)} \frac{\Delta_F}{\Delta_{\mathcal{E}}} \alpha(z)$$

We then have

$$\frac{\partial^2 \mathcal{L}}{\partial z^2} = (\mathcal{L} - z)^x (\mathcal{L} + z)^f$$

$$\mathcal{L} \sim z, \quad z \rightarrow \infty$$

$$\mathcal{L} \sim -z, \quad z \rightarrow -\infty$$

(6.15)

This is the same mathematical problem as obtained by Clarke (1967b)

and his predecessors. There appears to be no solution to this problem in terms of tabulated functions, and hence approximate or numerical solutions must be obtained.

### 6.3 Rayleigh-Ritz Approximation

Consider a variational method referred to as the Rayleigh-Ritz approximation. This means of approximation is discussed by Hildebrand (1965) for instance. Let  $\delta \mathcal{A}$  be the variation in the function  $\mathcal{A}$ . We now multiply the equation (6.15) by  $\delta \mathcal{A} dz$ , integrate over the whole range of  $z$ , and obtain

$$\int_{-\infty}^{\infty} \left[ \frac{\partial^2 \mathcal{A}}{\partial z^2} - (\mathcal{A} - z)^x (\mathcal{A} + z)^f \right] \delta \mathcal{A} dz = 0 \quad (6.16)$$

The first term may be integrated by parts. The integrated part vanishes when  $\delta \mathcal{A}$  vanishes at the end points, that is, when  $\mathcal{A}$  is fixed at the end points. We then get

$$\delta \int_{-\infty}^{\infty} \left[ \frac{1}{2} \left( \frac{\partial \mathcal{A}}{\partial z} \right)^2 + G(\mathcal{A}, z) \right] dz = 0 \quad (6.17)$$

where

$$G(\mathcal{A}, z) \equiv \int_0^{\mathcal{A}} (\lambda - z)^x (\lambda + z)^f d\lambda$$

The function  $\mathcal{A}(z)$  is such that the integral in (6.17) is an extremum.

In the Rayleigh-Ritz approximation, we choose a function that satisfies the boundary conditions on  $\mathcal{A}$  and that has several free parameters that are to be determined such that (6.16) or

(6.17) is satisfied for the function chosen. Here we choose a piecewise continuous function as follows:

$$\begin{aligned} \mathcal{A} = \mathcal{A}_1 &= -z + a^{-1} e^{b_1 z}, & z \leq 0 \\ \mathcal{A} = \mathcal{A}_2 &= z + a^{-1} e^{-b_2 z}, & z \geq 0 \end{aligned} \quad (6.18)$$

This satisfies the boundary conditions in (6.15) and is continuous at  $z=0$ . We further require that the derivative  $\frac{\partial \mathcal{A}}{\partial z}$  is continuous at  $z=0$ . This leads to

$$a = \frac{1}{2} (b_1 + b_2) \quad (6.19)$$

There are thus two constants to be determined,  $b_1$  and  $b_2$ . When  $\mathcal{X}$  and  $f$  are unequal, then  $b_1$  and  $b_2$  will be unequal, which reflects the asymmetry in  $\mathcal{A}$  for positive and negative  $z$ . When  $\mathcal{X}$  and  $f$  are equal, it should transpire from the analysis that  $b_1$  and  $b_2$  are equal.

The variation of  $\mathcal{A}$  is

$$\delta \mathcal{A} = \delta \mathcal{A}_1 = -\frac{1}{2a^2} [(1-2az)\delta b_1 + \delta b_2] e^{b_1 z}, \quad z \leq 0 \quad (6.20)$$

$$\delta \mathcal{A} = \delta \mathcal{A}_2 = -\frac{1}{2a^2} [\delta b_1 + (1+2az)\delta b_2] e^{-b_2 z}, \quad z \geq 0$$

We now substitute (6.18) and (6.20) into (6.16), collect coefficients of  $\delta b_1$  and  $\delta b_2$ , and set the collected coefficients equal to zero separately since  $\delta b_1$  and  $\delta b_2$  are arbitrary. This gives two equations for  $b_1$  and  $b_2$ , which we can arrange to read



$$\frac{3}{2} a^{1+x+f} = \frac{a}{b_1} \int_0^{\infty} \left(1 + \frac{2a}{b_1} y\right) \left(\frac{2a}{b_1} y + e^{-y}\right)^x e^{-(1+f)y} dy$$

$$+ \frac{a}{b_2} \int_0^{\infty} \left(\frac{2a}{b_2} y + e^{-y}\right)^f e^{-(1+x)y} dy$$

(6.21)

$$\left(\frac{a}{b_1}\right)^2 \int_0^{\infty} y \left(\frac{2a}{b_1} y + e^{-y}\right)^x e^{-(1+f)y} dy$$

$$= \left(\frac{a}{b_2}\right)^2 \int_0^{\infty} y \left(\frac{2a}{b_2} y + e^{-y}\right)^f e^{-(1+x)y} dy$$

(6.22)

Since

$$\frac{a}{b_2} = \frac{a/b_1}{2 \frac{a}{b_1} - 1}$$

(6.23)

equation (6.22) amounts to a single equation for  $\frac{a}{b_1}$  or  $\frac{a}{b_2}$ . After it has been solved, the right-hand side of (6.21) can be evaluated and  $a$  determined, and hence  $b_1$  and  $b_2$  can be determined.

When  $x=f=n$ , equation (6.22) yields that  $a=b_1=b_2$ , and equation (6.21) becomes

$$a^{1+2n} = \frac{4}{3} \int_0^{\infty} (1+y) (2y + e^{-y})^n e^{-(1+n)y} dy$$

(6.24)

The solution (6.18) can be written

$$\mathcal{L} = |z| + a^{-1} e^{-a|z|}$$

(6.25)

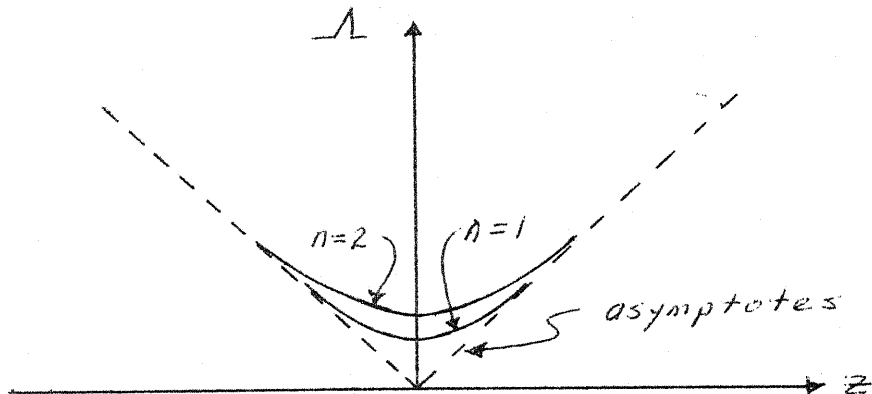
When  $n=1$  and  $2$ , we obtain

$$n=1 \quad a = \left(\frac{52}{27}\right)^{1/3} \approx 1.243$$

$$n=2 \quad a = \left(\frac{6521}{4050}\right)^{1/5} \approx 1.101$$

The minimum value of  $\mathcal{L}$  occurs when  $z=0$  for the symmetric case,  $x=f=n$ . The minimum value of  $\mathcal{L}$ , which according to (6.25) is  $a^{-1}$ , increases as the order of the reaction,  $n$ , increases.

The exponential term,  $\exp(-a/|z|)$ , governs the width of the flame. We see that the width of the flame increases as  $n$  increases. These features are depicted in Sketch 7.



Sketch 7. Dependence of  $\mathcal{L}$  on  $n$ , for  $x=f=n$ .

Consider now the asymmetric problem when  $x \neq f$ . We choose  $x=1$  and  $f=2$ , and (6.22) becomes

$$\left(\frac{a}{b_1}\right)^2 \left[ \frac{1}{16} + \frac{4}{27} \frac{a}{b_1} \right] = \left(\frac{a}{b_2}\right)^2 \left[ \frac{1}{16} + \frac{8}{27} \frac{a}{b_2} + \frac{3}{2} \left(\frac{a}{b_2}\right)^2 \right] \quad (6.26)$$

With relation (6.23) equation (6.26) is a higher-order polynomial for  $\frac{a}{b_1}$ . It can be solved graphically or by other numerical means. We determine that

$$\frac{a}{b_1} = 1.50 \quad , \quad \frac{a}{b_2} = 0.75$$

The value of  $a$  may now be determined from (6.21). We obtain

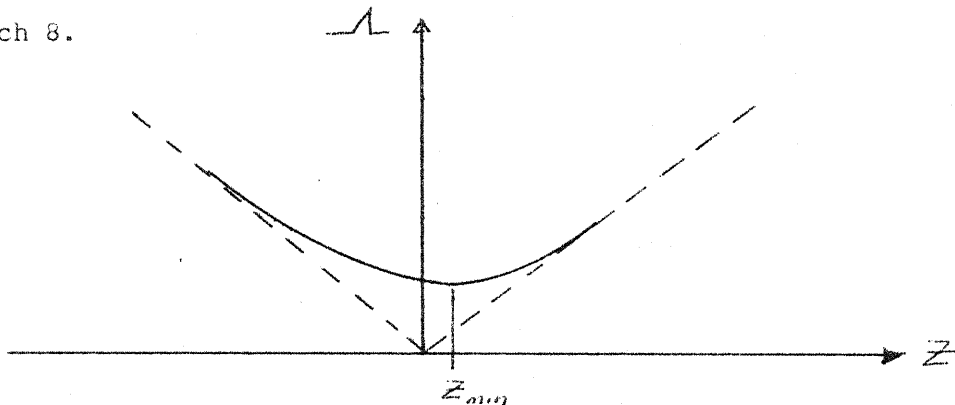
$a = 1.18$ . It thus follows that

$$\chi = 1, f = 2 : \quad a = 1.18 \quad , \quad b_1 = 0.79 \quad , \quad b_2 = 1.58$$

Further we may deduce that, if the values of  $\chi$  and  $f$  are interchanged,

$$\chi = 2, f = 1 : \quad a = 1.18 \quad , \quad b_1 = 1.58 \quad , \quad b_2 = 0.79$$

From the above Rayleigh-Ritz approximation we can now determine for  $\chi = 1, f = 2$ , that the minimum of  $\mathcal{A}$  is 0.818 and it is shifted to the point  $z = 0.168$ . When  $\chi = 2$  and  $f = 1$ , the minimum is the same, but shifted to  $z = -0.168$ . The curve approaches its asymptote rapidly on the side of the minimum, but more slowly on the opposite side. The curve is illustrated in Sketch 8.



Sketch 8. Asymmetry of  $\mathcal{A}$  for  $\chi = 1, f = 2$ .

It may be possible to obtain better Rayleigh-Ritz approximations by a more judicious selection of a trial function than (6.18). Nevertheless, the present approximation allows trends to be established for the different values of  $\lambda$  and  $f$ . Further work along these lines may be worthwhile.

#### 6.4 The Remaining Problem for the Flame Structure

The problem for the remaining variables can be investigated by first writing the continuity, momentum, and energy equations in terms of the inner coordinate  $Y$ . With the functions in terms of the inner coordinate written as  $\rho' = R(Y, \tau)$ ,  $p' = P(Y, \tau)$ ,  $T' = \Theta(Y, \tau)$ ,  $C' = G(Y, \tau)$ , and  $u' = U(Y, \tau)$ , we have

$$\epsilon^m \frac{\partial R'}{\partial \tau} + \frac{\partial U}{\partial Y} = 0 \quad (6.27)$$

$$\epsilon^{2m} \frac{\partial U}{\partial \tau} = -\frac{\epsilon^m}{\delta} \frac{\partial P}{\partial Y} + \frac{\partial^2 U}{\partial Y^2} \quad (6.28)$$

$$\epsilon^{2m} P_r \left( \frac{\partial \Theta}{\partial \tau} - \frac{\gamma-1}{\delta} \frac{\partial P}{\partial \tau} \right) = \frac{\partial^2 \Theta}{\partial Y^2} + \epsilon^{2m-1} P_r Q C_X^\lambda C_F^f \quad (6.29)$$

The linearized equation of state appears the same as before:

$$P = R + \Theta + \alpha_F C_F + \alpha_X C_X \quad (6.30)$$

We now assume expansions of the form

$$\begin{aligned} P &\sim P_0 + \epsilon^m P_1 + \epsilon^{2m} P_2 + \dots \\ R &\sim R_0 + \epsilon^m R_1 + \epsilon^{2m} R_2 + \dots \\ \Theta &\sim \Theta_0 + \epsilon^m \Theta_1 + \epsilon^{2m} \Theta_2 + \dots \\ U &\sim U_0 + \epsilon^m U_1 + \epsilon^{2m} U_2 + \dots \end{aligned} \quad (6.31)$$

The expansion for the concentrations are given by (6.3).

Substituting these expansions into the governing equations, collecting like powers of  $\epsilon^n$ , and requiring that these collected coefficients vanish lead to

$$\begin{aligned}
 \epsilon^0 : \quad & \left. \begin{aligned} \frac{\partial U_0}{\partial Y} &= 0 \\ \frac{\partial^2 U_0}{\partial Y^2} &= 0 \\ \frac{\partial^2 \Theta_0}{\partial Y^2} &= 0 \\ P_0 &= R_0 + \Theta_0 \end{aligned} \right\} \quad (6.32)
 \end{aligned}$$

$$\begin{aligned}
 \epsilon^1 : \quad & \left. \begin{aligned} \frac{\partial R_0}{\partial \xi} + \frac{\partial U_1}{\partial Y} &= 0 \\ -\frac{1}{\delta} \frac{\partial P_0}{\partial Y} + \frac{\partial^2 U_1}{\partial Y^2} &= 0 \\ \frac{\partial^2 \Theta_1}{\partial Y^2} + P_1 Q C_{X1}^x C_{F1}^f &= 0 \\ P_1 &= R_1 + \Theta_1 + \delta_X C_{X1} + \delta_F C_{F1} \end{aligned} \right\} \quad (6.33)
 \end{aligned}$$

Equations (6.32) plus the first two equations of (6.33) together with the matching conditions yield that the zeroth-order inner functions are simply the outer functions evaluated on the flame sheet. (See section 4.7). Hence we have

$$\begin{aligned}
 U_0 &= u'(0, \xi) \\
 R_0 &= f'(0, \xi) \\
 P_0 &= p'(0, \xi) \\
 \Theta_0 &= T'(0, \xi)
 \end{aligned} \quad \left. \right\} \quad (6.34)$$

Here we should realize that the outer solution, analyzed previously, is actually the linearized zeroth-order approximation for the outer expansion. At this stage we further deduce that the first-order velocity is given by

$$U_1(Y, \delta) = - \frac{\partial f'}{\partial \delta}(0, \delta) Y \quad (6.35)$$

It may be verified that this matches with the outer zeroth-order solution.

The functions  $e_{S1}$  and  $e_{F1}$  can be regarded as known. Hence the first-order inner temperature is determined by the third equation in (6.33). To obtain a closed system of equations for the first-order problem, we need the first two equations for the expansion corresponding to  $\epsilon^{2m}$ , which are obtained from the continuity and momentum equations:

$$\begin{aligned} \frac{\partial R_1}{\partial \delta} + \frac{\partial U_2}{\partial Y} &= 0 \\ \frac{\partial U_0}{\partial \delta} &= - \frac{1}{\delta} \frac{\partial R_1}{\partial Y} + \frac{\partial^2 U_2}{\partial Y^2} \end{aligned} \quad (6.36)$$

The last two equations of (6.34) together with (6.36) provide four equations for  $R_1$ ,  $P_1$ ,  $\Theta_1$ , and  $U_2$ .

### 6.5 The Temperature in the Flame

When the factor  $c_{X1}^x c_{F1}^f$  is eliminated between equation (6.5) and the third of equations (6.33) we obtain

$$\frac{\partial^2 \Theta_1}{\partial Y^2} = - \frac{P_r Q}{S_c \alpha W_X} \frac{\partial^2 c_{X1}}{\partial Y^2} \quad (6.37)$$

A first integration gives

$$\frac{\partial \Theta_1}{\partial Y} = - \frac{P_r Q}{S_c \alpha W_X} \frac{\partial c_{X1}}{\partial Y} + b_0(\tau) \quad (6.38)$$

where  $b_0(\tau)$  is a function of integration. Matching with the outer solution yields that

$$b_0(\tau) = \frac{\partial T'}{\partial X}(0^+, \tau) \quad (6.39)$$

$$\sim - \frac{1}{2} \sqrt{\frac{P_r}{\pi \tau}} \left[ \Delta_T - \frac{\gamma-1}{\delta} \Delta_p + \sqrt{\frac{P_r}{S_c}} \frac{\Delta_X Q}{\alpha W_X} \right], \quad \tau \rightarrow \infty$$

A second integration gives

$$\Theta_1 = - \frac{P_r Q}{S_c \alpha W_X} c_{X1} + b_0(\tau) Y, \quad (6.40)$$

where the second function of integration is found to vanish by virtue of matching. Thus the temperature function  $\Theta_1$  is determined in terms of the concentration function,  $c_{X1}$ , which has already been analyzed.

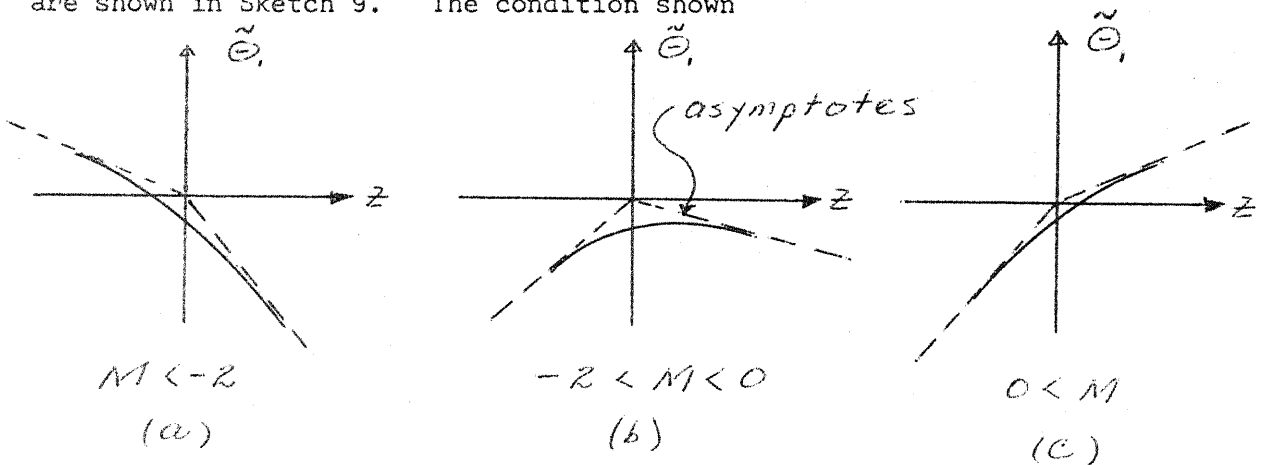
In terms of the function  $\mathcal{L}$  and the coordinate  $z$ , defined by (6.14), the temperature  $\Theta_i$ , can be expressed as

$$\frac{s'_c \times W_I}{P_r Q} \frac{\Theta_i}{\Delta(T)} \equiv \tilde{\Theta}_i = -\mathcal{L} + (1+M)z, \quad (6.41)$$

where

$$M \equiv \frac{2b_0 \Delta_F}{a_0 \Delta_I} \frac{s'_c \times W_I}{P_r Q}$$

Since for large time  $M$  does not depend on  $\tau$ ,  $\tilde{\Theta}_i$  can be plotted as a function of only  $z$  for large time. The shape of the curve will depend on the values of the initial conditions which determine the value of  $M$ . The three possible conditions are shown in Sketch 9. The condition shown



Sketch 9. Temperature Profiles in the Flame.

by Sketch 9b corresponds to an outer temperature distribution as illustrated by Fig. 4.



### 6.6 Pressure, Density, and Velocity in the Flame

The second of equations (6.36) can be integrated once to give the pressure function as

$$P_1 = \gamma \left[ - \frac{\partial U'}{\partial \tau}(0, \tau) Y + \frac{\partial U_2}{\partial Y} \right] \quad (6.42)$$

The function of integration was found to vanish because of matching. Elimination of the velocity derivative by means of the first of equations (6.36) yields

$$P_1 = -\gamma \left[ \frac{\partial U'}{\partial \tau}(0, \tau) Y + \frac{\partial R_1}{\partial \tau} \right] \quad (6.43)$$

Substitution of this expression into the last of equations (6.33) yields a first-order differential equation for  $R_1$ , since the temperature and concentrations can be regarded as known. Integration then gives

$$R_1 = -e^{-\tau} \int_0^{\tau} e^{\tau} \left[ Y \frac{\partial U'}{\partial \tau}(0, \tau) + \Theta_1 + \gamma_S C_{S1} + \gamma_F C_{F1} \right] d\tau \quad (6.44)$$

Examination of the functions involved in the above expressions shows that the pressure dies out faster with time than the density, temperature, or concentration. Hence for large time the density is given approximately by

$$R_1 \sim - \left[ \Theta_1 + \gamma_S C_{S1} + \gamma_F C_{F1} \right], \quad \tau \rightarrow \infty \quad (6.45)$$

Accordingly the pressure is determined by (6.43).

The velocity is obtained by integrating the first of equations

(6.36):

$$U_2 = - \int_0^Y \frac{\partial R_1}{\partial \tau} dY \quad (6.46)$$

The function of integration vanishes because of matching.

### 6.7 Composite Expansions

It is useful to represent the entire flow field by a uniformly valid approximation called a composite expansion. Let  $\Phi$  represent a function and  $\Phi^{(o)}$  and  $\Phi^{(i)}$  its outer and inner expansions.

Let  $\Phi^{(cp)}$  represent the common part of the inner and outer expansion, that is, the parts that match. The additive method of forming a composite solution is (see Van Dyke 1964)

$$\Phi^{(c)} = \Phi^{(o)} + \Phi^{(i)} - \Phi^{(cp)}$$

For the temperature perturbation, we have to the order of our present analysis

$$\begin{aligned} T^{(c)} &= T'(x, \tau) + [\Theta_o + \epsilon^n \Theta_i] \\ &\quad - [\Theta_o + T_x^{(cp)} x] \\ &= T'(x, \tau) + \epsilon^n \Theta_i(\gamma, \tau) - T_x^{(cp)} x, \end{aligned} \quad (6.47)$$

where

$$\begin{aligned} T_x^{(cp)} &= \frac{\partial T'}{\partial x}(0^+, \tau), \quad x > 0 \\ &= \frac{\partial T'}{\partial x}(0^-, \tau), \quad x < 0 \end{aligned} \quad (6.48)$$

The composite solution is continuous in the first derivative.

Similar results can be written for the other variables.

### 6.8 Thickness of the Flame

The zone of significant reactions ceases when the inner solution merges with the outer. The function that governs the inner region, the flame, is  $\mathcal{L}$ . The width of the flame can be specified by selecting some arbitrary value of  $\bar{z}$ , say  $\bar{z}_f$ , which indicates where  $\mathcal{L}$  merges with  $\bar{z}$ , the asymptotic value. The physical thickness of the flame,  $\Delta Y_f$ , is related to  $\Delta \bar{z}_f$  by means of (6.14).

We thus have

$$\begin{aligned} \Delta Y_f &= \beta \Delta \bar{z}_f \\ &= \left\{ \frac{a_0(\bar{t})}{\mathcal{L}} \frac{\Delta \bar{x}}{\Delta F} \right\}^{2m-1} \left\{ \frac{\Delta \bar{x}}{\Delta F} \frac{1}{\chi W_X S'_c} \right\} \Delta \bar{z}_f \end{aligned}$$

As shown by (6.10),  $a_0$  varies like  $\bar{t}^{-1/2}$ , and hence  $\Delta Y_f$  varies like  $\bar{t}^{1/2-m}$ . Since  $m$  is always less than or equal to  $1/3$ , the flame thickness is thus seen to increase with time. Correspondingly, however, the intensity of the flame, associated with the amplitude of  $\bar{e}_{x1}$ , at  $\bar{z}=0$ , decreases with time, as might be expected since the flame strength,  $\bar{S}$ , decreases with time.

It is interesting to compare the present unsteady case with the somewhat analogous two dimensional steady flame studied by Clarke (1967b). In terms of the parabolic coordinate measured normal to the flame,  $\mathcal{V}$ , the width of the flame in Clarke's problem was found to decrease in the downstream direction. The physical distance measured normal to the flame, however, is determined by  $ds_{\mathcal{V}} = h_{\mathcal{V}} d\mathcal{V}$ , where  $h_{\mathcal{V}}$  is the appropriate scale factor. When this is taken into account, it is found that the width of the flame in Clarke's problem also increases downstream, and in a fashion directly analogous to the unsteady problem considered here.

7. CONCLUDING REMARKS

An analysis for a diffusion flame associated with a weak explosion, the one-dimensional shock-tube problem, has been treated in some detail. Further work along these lines would be valuable. With continued use of the linearized theory, the results for non-stoichiometric initial conditions should be carried out. This would provide a flow field associated with a moving flame.

It would also be very informative to deal with this problem on a nonlinear basis, at least for slightly stronger explosions if not for intense explosions. Hopefully the results of the linear analysis can shed light on how to approach the more complicated nonlinear problem. It may be worthwhile to consider Lagrangian coordinates as an alternative to the Eulerian coordinates.

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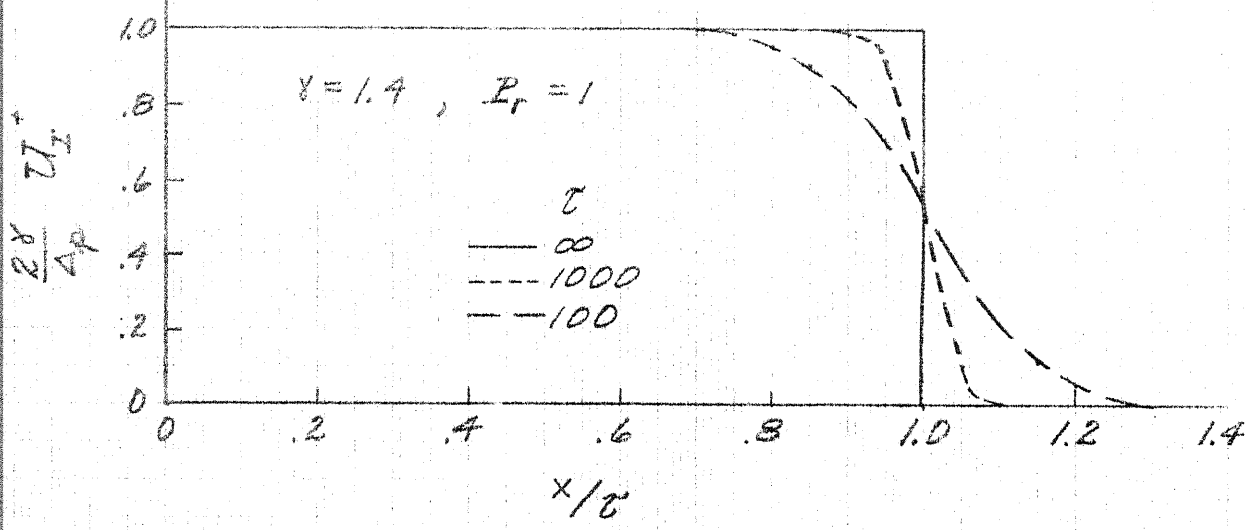


FIG. 1 PRESSURE INDUCED VELOCITY WAVE

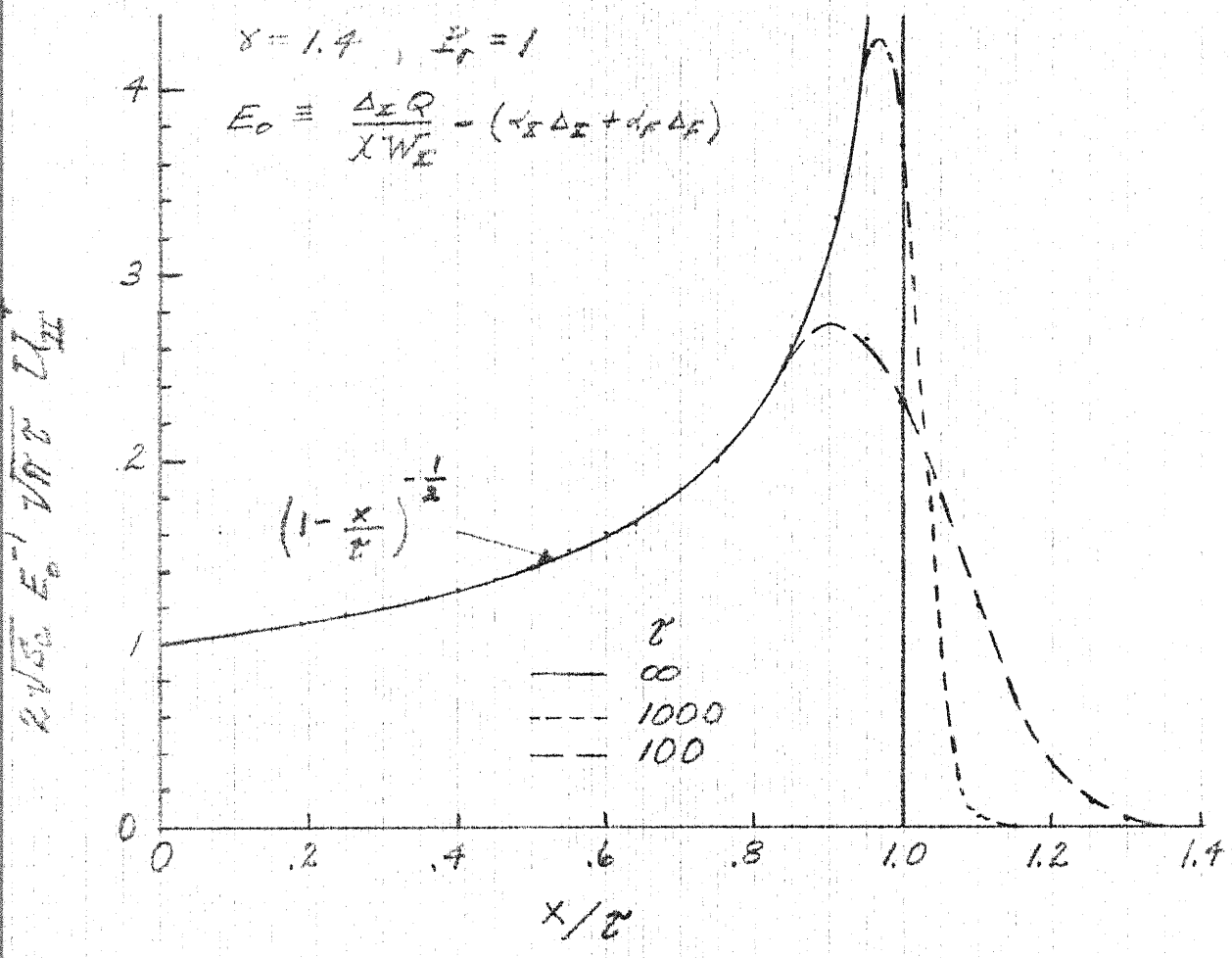


FIG. 2 FLAME INDUCED VELOCITY WAVE

R.P. N<sup>-1</sup> V<sup>2</sup> U<sub>max</sub><sup>+</sup>

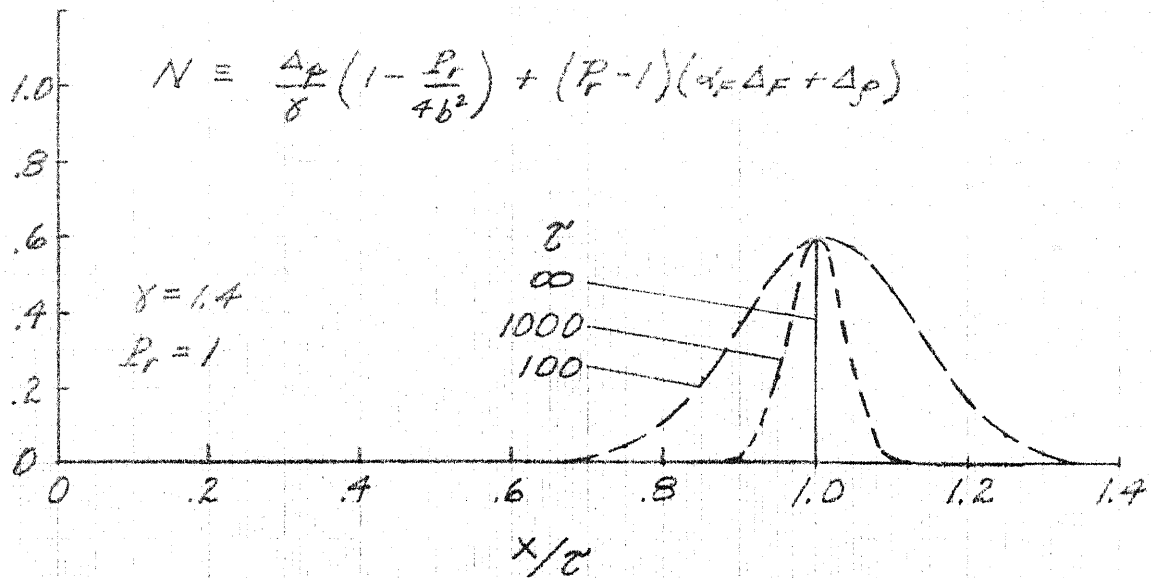


FIG. 3 VELOCITY CONTRIBUTION  $U_{III}^+$



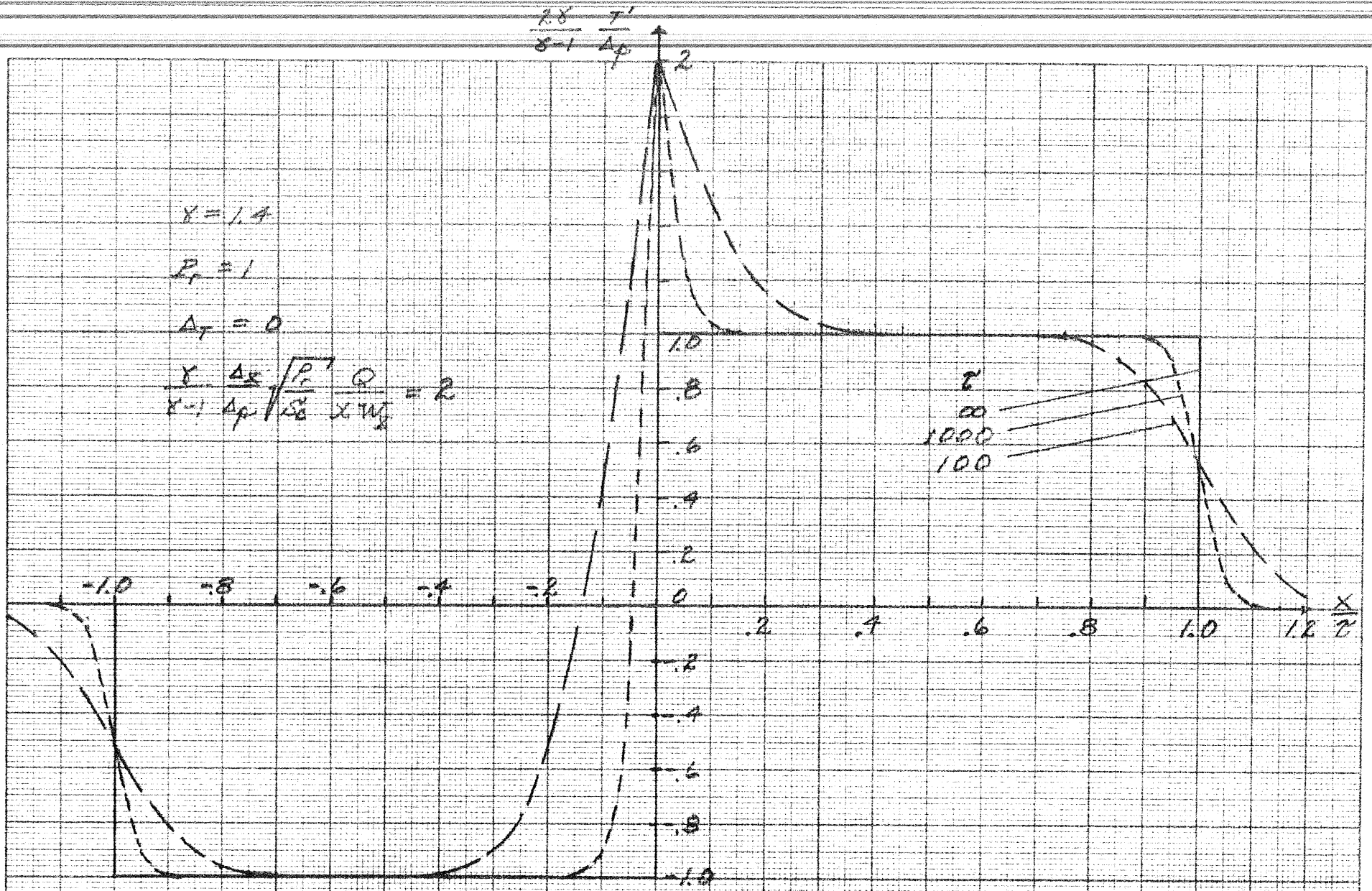
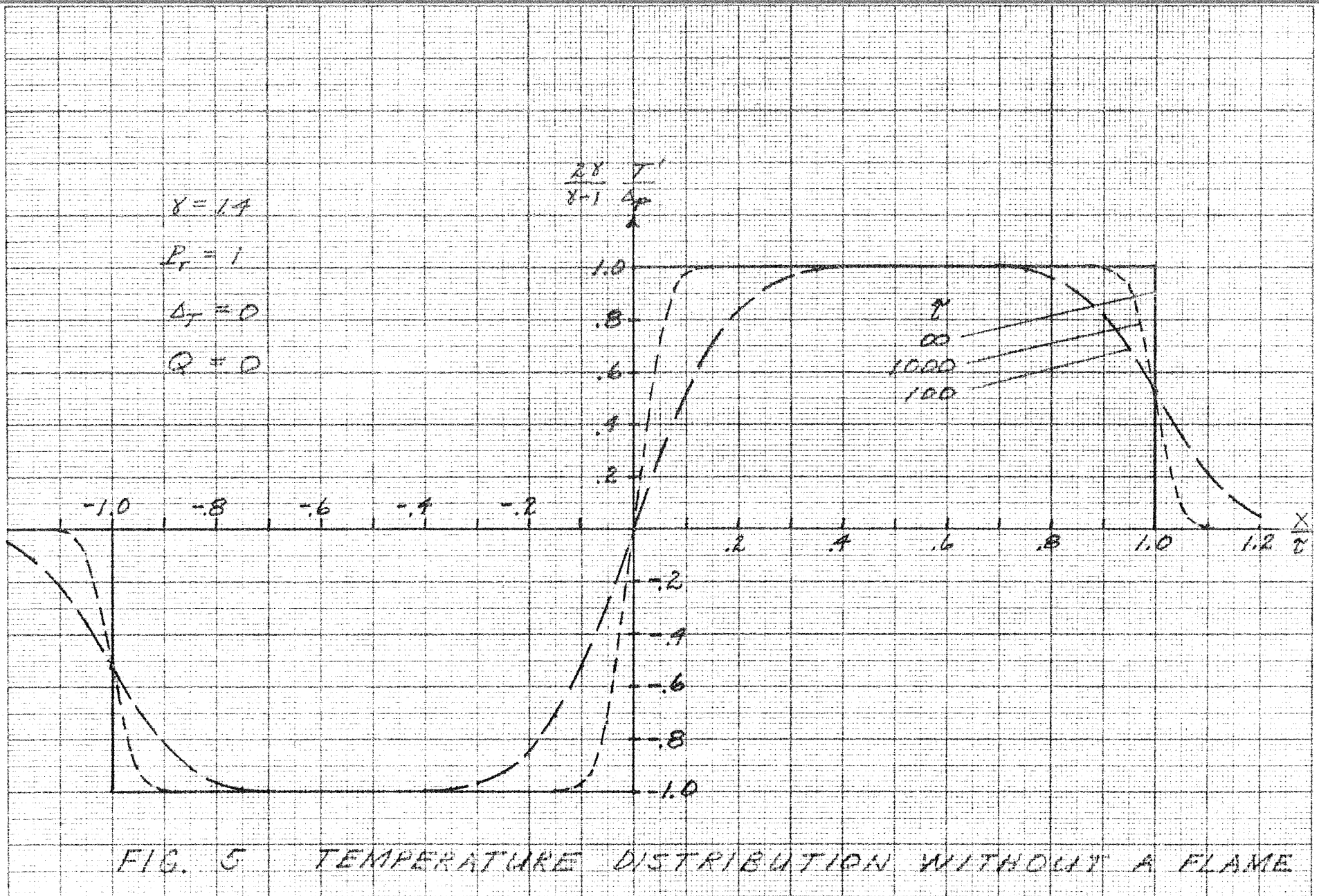


FIG. 4. TEMPERATURE DISTRIBUTION WITH A FLAME



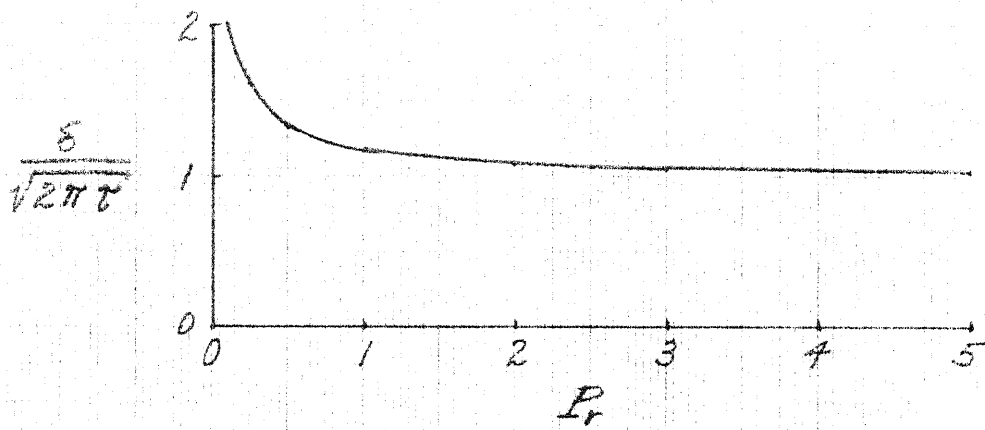


FIG. 6 WAVE THICKNESS VS.  $Pr$

APPENDIX A

CONSTITUTIVE RELATIONS FOR THE DIFFUSION-FLUX

AND HEAT-FLUX VECTORS

We consider a reacting mixture of  $n$  species of gases. We assume small departures from equilibrium so that the change of entropy of a fluid particle is described by the thermodynamical relation

$$T \frac{DS}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} - \sum_{\alpha=1}^n \mu_{\alpha} \frac{DC_{\alpha}}{Dt} \quad (A.1)$$

where  $\mu_{\alpha}$  is the chemical potential of species  $\alpha$  and  $C_{\alpha}$  is the mass fraction of species  $\alpha$ . The mass fractions are not all independent since they must satisfy the relation

$$\sum_{\alpha=1}^n C_{\alpha} = 1 \quad (A.2)$$

We thus arbitrarily select the first  $n-1$  mass fractions as independent and determine  $C_n$  from (A.2). Thus equation (A.1) may be rewritten as

$$T \frac{DS}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} - \sum_{\alpha=1}^{n-1} \tilde{\mu}_{\alpha} \frac{DC_{\alpha}}{Dt} \quad (A.2)$$

where

$$\begin{aligned} \tilde{\mu}_{\alpha} &\equiv \mu_{\alpha} - \mu_n \\ &= \tilde{\mu}_{\alpha}(p, T, c_1, c_2, \dots, c_{n-1}) \end{aligned} \quad (A.3)$$

The energy equation can be written

$$\rho \frac{Dh}{Dt} = \frac{DP}{Dt} + \vec{T} : \vec{E} - \text{div} \vec{q} \quad (\text{A.4})$$

where  $\vec{T}$  is the viscous stress tensor,  $\vec{E}$  the rate of strain tensor, and  $\vec{q}$  the heat-flux vector. The equations of change for the mass fractions  $c_\alpha$  are

$$\rho \frac{Dc_\alpha}{Dt} = -\text{div} \vec{f}_\alpha + \rho K_\alpha, \quad \alpha = 1, 2, \dots, n. \quad (\text{A.5})$$

Here  $\vec{f}_\alpha$  is the diffusion-flux vector for species  $\alpha$  and  $K_\alpha$  is the mass rate of production of species  $\alpha$  per unit mass. The production rates,  $K_\alpha$ , and the vectors,  $\vec{f}_\alpha$ , are not all independent for they must satisfy the relations

$$\sum_{\alpha=1}^n \vec{f}_\alpha = 0 \quad \text{and} \quad \sum_{\alpha=1}^n K_\alpha = 0. \quad (\text{A.6})$$

We can regard the first  $n-1$  components as independent.

If we now eliminate  $Dh/Dt$  and  $Dc_\alpha/Dt$  in eq. (A.2) by means of (A.4) and (A.5) we obtain for the rate of change of entropy of a fluid particle

$$\rho \frac{DS}{Dt} = \frac{\vec{T} : \vec{E}}{T} - \frac{\rho}{T} \sum_{\alpha=1}^{n-1} \tilde{M}_\alpha K_\alpha + \frac{1}{T} \sum_{\alpha=1}^{n-1} \tilde{M}_\alpha \text{div} \vec{f}_\alpha - \frac{1}{T} \text{div} \vec{q} \quad (\text{A.7})$$

The fluxes of entropy to the fluid particle are more clearly

portrayed if we rewrite Eq. (A.7) as

$$\rho \frac{DS}{Dt} = \frac{\vec{\tau} : \vec{E}}{T} - \frac{\rho}{T} \sum_{\alpha=1}^{n-1} \mu_{\alpha}^{\sim} K_{\alpha} - \frac{1}{T} \sum_{\alpha=1}^{n-1} \vec{f}_{\alpha} \cdot \nabla \mu_{\alpha}^{\sim} - \frac{1}{T^2} \left( \vec{q} - \sum_{\alpha=1}^{n-1} \mu_{\alpha}^{\sim} \vec{f}_{\alpha} \right) \cdot \nabla T - \text{div} \left[ \frac{\vec{q} - \sum_{\alpha=1}^{n-1} \mu_{\alpha}^{\sim} \vec{f}_{\alpha}}{T} \right] \quad (\text{A.8})$$

The divergence term on the right-hand side of (A.8) is a flux term, and the remaining terms on the right-hand side are source terms, or production terms. In accordance with the principles underlying the second law of Thermodynamics, we require that source terms be positive for all variations of the independent variables involved. This sort of principle underlies the Clausius-Duhem inequality in continuum mechanics (see Eringen (1967), for instance.) Green and Laws (1971) utilize such a principle in dealing with global properties of mixtures. Here our approach is akin to that for binary mixtures discussed by Landau and Lifshitz (1959). The constitutive relations must be devised such that entropy production is positive. For the Navier-Stokes stress relation

$$\vec{\tau} = 2\mu \vec{E} + \lambda (\text{div } \vec{v}) \underline{\underline{I}}$$

$$\vec{E} \equiv \frac{1}{2} \left[ \nabla \vec{v} + (\nabla \vec{v})^t \right] \quad (\text{A.9})$$

the viscous dissipation term  $\vec{\tau} : \vec{E}$  is found to be positive definite provided that  $\mu$  is positive and  $(\lambda + \frac{2}{3}\mu)$  is

positive. Likewise, the species mass production rates per unit mass,  $K_d$ , must satisfy the inequality

$$-\sum_{d=1}^{n-1} \tilde{\mu}_d K_d > 0 \quad . \quad (A.10)$$

The remaining source terms on the right-hand side of (A.8) can be used to establish conditions on the diffusion-flux vectors,  $\vec{J}_d$ , and the heat-flux vector,  $\vec{q}$ .

The third and fourth terms on the right side of (A.8) describe entropy production due to mass and heat diffusion. They involve  $\vec{J}_d$ ,  $\vec{q}$ ,  $\tilde{\mu}_d$ , and  $T$ . It is reasonable to assume that  $\vec{J}_d$  and  $\vec{q}$  depend on gradients of  $\tilde{\mu}_d$  and  $T$ , at least for first order. Hence we assume the following forms:

$$\vec{J}_d = -\sum_{\beta=1}^{n-1} A_{d\beta} \nabla \tilde{\mu}_\beta - B_d \nabla T, \quad d=1,2,\dots,n-1 \quad (A.11)$$

$$\vec{q} - \sum_{d=1}^{n-1} \tilde{\mu}_d \vec{J}_d = -\sum_{d=1}^{n-1} E_d \nabla \tilde{\mu}_d - F \nabla T \quad (A.12)$$

We now must establish conditions on the parameters  $A_{\alpha\beta}$ ,  $B_d$ ,  $E_d$ , and  $F$  such that the entropy production is positive definite. Out of the vectors,  $\vec{q}$ ,  $\vec{J}_d$ ,  $\nabla \tilde{\mu}_d$ , and  $\nabla T$ , we choose  $\vec{J}_d$  and  $\nabla T$  to be independent since

when there is no diffusion only  $\nabla T$  should influence the heat flux and not  $\nabla \tilde{\mu}_d$ . Hence we solve for  $\nabla \tilde{\mu}_d$  in terms of  $\vec{j}_d$  and  $\nabla T$  in (A.11). We obtain

$$\nabla \tilde{\mu}_d = - \sum_{\beta=1}^{n-1} A_{d\beta}^{-1} (\vec{j}_\beta + B_\beta \nabla T), \quad d=1,2,\dots,n-1, \quad (\text{A.13})$$

where  $A_{d\beta}^{-1}$  is the element of the inverse of the matrix  $\{A_{d\beta}\}$ . Eq. (A.12) now becomes

$$\vec{q} - \sum_{d=1}^{n-1} \tilde{\mu}_d \vec{j}_d = \sum_{\beta=1}^{n-1} \omega_\beta \vec{j}_\beta - \left( F - \sum_{\beta=1}^{n-1} \omega_\beta B_\beta \right) \nabla T \quad (\text{A.14})$$

$$\text{where} \quad \omega_\beta \equiv \sum_{d=1}^{n-1} E_d A_{d\beta}^{-1} \quad (\text{A.15})$$

When (A.13) and (A.14) are substituted into the third and fourth entropy production terms in (A.8), we obtain

$$\begin{aligned} -\frac{1}{T} \sum_{d=1}^{n-1} \vec{j}_d \cdot \nabla \tilde{\mu}_d - \frac{1}{T^2} \left( \vec{q} - \sum_{d=1}^{n-1} \tilde{\mu}_d \vec{j}_d \right) \cdot \nabla T &= \sum_{d=1}^{n-1} \sum_{\beta=1}^{n-1} \frac{A_{d\beta}^{-1}}{T} \vec{j}_d \cdot \vec{j}_\beta \\ &+ \sum_{d=1}^{n-1} \left( \sum_{\beta=1}^{n-1} \frac{A_{d\beta}^{-1} B_\beta}{T} - \frac{\omega_d}{T^2} \right) \vec{j}_d \cdot \nabla T + \left( F - \sum_{\beta=1}^{n-1} \omega_\beta B_\beta \right) (\nabla T)^2 \end{aligned} \quad (\text{A.16})$$

In order for (A.16) to be positive definite for independent variations of  $\vec{j}_d$  and  $\nabla T$ , we must have

$$A_{dd}^{-1} > 0 \quad (\text{A.17})$$



$$A_{\alpha\beta}^{-1} = -A_{\beta\alpha}^{-1}, \quad \beta \neq \alpha \quad (\text{A.18})$$

$$\omega_\alpha = T \sum_{\beta=1}^{n-1} A_{\alpha\beta}^{-1} B_\beta \quad (\text{A.19})$$

$$F - \sum_{\beta=1}^{n-1} \omega_\beta B_\beta > 0 \quad (\text{A.20})$$

Expressions (A.17) and (A.18) require that the diagonal elements of the array  $\{A_{\alpha\beta}\}$  are positive but out of  $(n-1)^2$  elements only  $n(n-1)/2$  are independent, and the off diagonal elements are anti-symmetric. The thermal conductivity,  $k$ , can be identified as the positive quantity

$$k \equiv F - \sum_{\beta=1}^{n-1} \omega_\beta B_\beta, \quad (\text{A.21})$$

and we can now write the expressions for  $\vec{j}_\alpha$  and  $\vec{q}$  as

$$\vec{j}_\alpha = - \sum_{\beta=1}^{n-1} A_{\alpha\beta} \nabla \tilde{\mu}_\beta - B_\alpha \nabla T \quad (\text{A.22})$$

$$\vec{q} = -k \nabla T + \sum_{\alpha=1}^{n-1} \left( \tilde{\mu}_\alpha + T \sum_{\beta=1}^{n-1} A_{\alpha\beta}^{-1} B_\beta \right) \vec{j}_\alpha \quad (\text{A.23})$$

The diffusion vectors can be written in terms of gradients of  $c_\alpha$ ,  $p$ , and  $T$  if the functional relation (A.3) is recalled. We then have

$$\nabla \tilde{\mu}_\alpha = \sum_{\beta=1}^{n-1} \frac{\partial \tilde{\mu}_\alpha}{\partial c_\beta} \nabla c_\beta + \frac{\partial \tilde{\mu}_\alpha}{\partial p} \nabla p + \frac{\partial \tilde{\mu}_\alpha}{\partial T} \nabla T, \quad (\text{A.24})$$

$$\alpha = 1, 2, \dots, n-1$$

Equation (A.22) can now be written as

$$\vec{j}_d = - \sum_{\beta=1}^{n-1} \tilde{D}_{d\beta} \nabla C_{\beta} - D_d^{(p)} \nabla \ln p - D_d^{(T)} \nabla \ln T, \quad (\text{A.25})$$

$d = 1, 2, \dots, n-1$

where

$$\tilde{D}_{d\beta} \equiv \sum_{m=1}^{n-1} A_{dm} \frac{\partial \tilde{\mu}_m}{\partial C_{\beta}} \quad (\text{A.26})$$

multi-component

are diffusion coefficients and

$$D_d^{(T)} \equiv T \left( B_d + \sum_{\beta=1}^{n-1} A_{d\beta} \frac{\partial \tilde{\mu}_{\beta}}{\partial T} \right) \quad (\text{A.27})$$

$$D_d^{(p)} = p \sum_{\beta=1}^{n-1} A_{d\beta} \frac{\partial \tilde{\mu}_{\beta}}{\partial p}$$

are the thermal-diffusion and pressure-diffusion coefficients.

By simple matrix methods it is not difficult to show from

(A.27) that

$$T \sum_{\alpha=1}^{n-1} A_{\beta\alpha}^{-1} B_{\alpha} = -T \frac{\partial \tilde{\mu}_{\beta}}{\partial T} - \sum_{\alpha=1}^{n-1} A_{\beta\alpha}^{-1} D_{\alpha}^{(T)} \quad (\text{A.28})$$

Hence the heat-flux vector, (A.23), can be written

$$\vec{q} = -k \nabla T + \sum_{\alpha=1}^{n-1} \left( \tilde{\mu}_{\alpha} - T \frac{\partial \tilde{\mu}_{\alpha}}{\partial T} \right) \vec{j}_{\alpha} + \sum_{\alpha=1}^{n-1} \sum_{\beta=1}^{n-1} A_{\alpha\beta}^{-1} D_{\beta}^{(T)} \vec{j}_{\alpha} \quad (\text{A.29})$$

which is a form involving the thermal diffusion coefficients

and similar to a form found in kinetic theory.

The parameters  $A_{\alpha\beta}$  can be determined in terms of  $\tilde{D}_{\alpha\beta}$  by means of (A.26). Let  $M_{\alpha\beta} \equiv \frac{\partial \mu_{\alpha}}{\partial c_{\beta}}$ . Then in matrix notation (A.26) becomes

$$D = A M \quad , \quad (A.30)$$

and it follows that

$$\begin{aligned} A &= D M^{-1} \\ A^{-1} &= M D^{-1} \end{aligned} \quad (A.31)$$

One can also establish that

$$\tilde{\mu}_{\alpha} = \left( \frac{\partial g}{\partial c_{\alpha}} \right)_{T, p, c_{\beta}} \quad (A.32)$$

where  $g = h - TS$  is the Gibbs free enthalpy. It then can be shown that

$$\tilde{\mu}_{\alpha} - T \frac{\partial \tilde{\mu}_{\alpha}}{\partial T} = \left( \frac{\partial h}{\partial c_{\alpha}} \right)_{p, T, c_{\beta}} \quad (A.33)$$

For a mixture of thermally perfect gases, we have

$$\tilde{\mu}_{\alpha} - T \frac{\partial \tilde{\mu}_{\alpha}}{\partial T} = h_{\alpha}(T) \quad (A.34)$$

$$\frac{\partial \tilde{\mu}_{\alpha}}{\partial p} = \frac{T}{p} (R_{\alpha} - R_n) \quad (A.35)$$

$$M_{\alpha\beta} \equiv \frac{\partial \tilde{U}_\alpha}{\partial C_\beta} = T \left[ \frac{R_\alpha \delta_{\alpha\beta}}{C_\alpha} + \frac{R_\alpha}{C_\alpha} - \frac{(R_\alpha - R_\alpha)(R_\beta - R_\alpha)}{\sum_{m=1}^n R_m C_m} \right] \quad (\text{A.36})$$

Note that  $M_{\alpha\beta}$  is symmetric, and that  $R_\alpha = \frac{\kappa}{m_\alpha}$  is the specific gas constant. By means of (A.36),  $A_{\alpha\beta}$  can be determined in terms of the diffusion coefficients  $\tilde{D}_{\alpha\beta}$  with the use of (A.31).

Consider the special case of a ternary mixture of thermally perfect gases. Equation (A.31) can then be written

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \frac{1}{\det M} \begin{bmatrix} \tilde{D}_{11} & \tilde{D}_{12} \\ \tilde{D}_{21} & \tilde{D}_{22} \end{bmatrix} \begin{bmatrix} M_{22} & -M_{12} \\ -M_{12} & M_{11} \end{bmatrix} \quad (\text{A.37})$$

where

$$M_{11} = T \left[ \frac{R_1}{C_1} + \frac{R_3}{C_3} - \frac{(R_1 - R_3)^2}{R_1 C_1 + R_2 C_2 + R_3 C_3} \right] \quad (\text{A.38})$$

$$M_{12} = M_{21} = T \left[ \frac{R_3}{C_3} - \frac{(R_1 - R_3)(R_3 - R_3)}{R_1 C_1 + R_2 C_2 + R_3 C_3} \right] \quad (\text{A.39})$$

$$M_{22} = T \left[ \frac{R_2}{C_2} + \frac{R_3}{C_3} - \frac{(R_2 - R_3)^2}{R_1 C_1 + R_2 C_2 + R_3 C_3} \right] \quad (\text{A.40})$$

$$\det M = M_{11} M_{22} - M_{12}^2 \quad (\text{A.41})$$

Expansion of (A.37) yields

$$A_{11} = \frac{\tilde{D}_{11} M_{22} - \tilde{D}_{12} M_{12}}{M_{11} M_{22} - M_{12}^2} \quad (\text{A.42})$$

$$A_{12} = \frac{\tilde{D}_{12} M_{11} - \tilde{D}_{11} M_{12}}{M_{11} M_{22} - M_{12}^2} \quad (\text{A.43})$$

$$A_{21} = \frac{\tilde{D}_{21} M_{22} - \tilde{D}_{22} M_{12}}{M_{11} M_{22} - M_{12}^2} \quad (\text{A.44})$$

$$A_{22} = \frac{\tilde{D}_{22} M_{11} - \tilde{D}_{21} M_{12}}{M_{11} M_{22} - M_{12}^2} \quad (\text{A.45})$$

Since  $A_{12} = -A_{21}$  by virtue of (A.18), the coefficients  $\check{D}_{11}$ ,  $\check{D}_{12}$ ,  $\check{D}_{21}$ ,  $\check{D}_{22}$  are not all independent and are related by

$$\check{D}_{12} M_{11} - \check{D}_{11} M_{12} = \check{D}_{22} M_{12} - \check{D}_{21} M_{22} \quad (A.46)$$

The pressure-diffusion coefficients, (A.27), depend on the diffusion coefficients  $\check{D}_{\alpha\beta}$  as follows:

$$D_1^{(p)} = T [A_{11}(R_1 - R_3) + A_{12}(R_2 - R_3)] \quad (A.47)$$

$$= \frac{T [\check{D}_{11} \{ (R_1 - R_3) M_{22} - (R_2 - R_3) M_{12} \} + \check{D}_{12} \{ (R_2 - R_3) M_{11} - (R_1 - R_3) M_{12} \}]}{M_{11} M_{22} - M_{12}^2}$$

$$D_2^{(p)} = T [A_{21}(R_1 - R_3) + A_{22}(R_2 - R_3)] \quad (A.48)$$

$$= \frac{T [\check{D}_{22} \{ (R_2 - R_3) M_{11} - (R_1 - R_3) M_{12} \} + \check{D}_{21} \{ (R_1 - R_3) M_{22} - (R_2 - R_3) M_{12} \}]}{M_{11} M_{22} - M_{12}^2}$$

To compute the Dufour effect, that is, the third term on the right-hand side of (A.29), we need to evaluate  $A_{\alpha\beta}^{-1}$ .

From (A.31) we have

$$\begin{bmatrix} A_{11}^{-1} & A_{12}^{-1} \\ A_{21}^{-1} & A_{22}^{-1} \end{bmatrix} = \frac{1}{\det D} \begin{bmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{bmatrix} \begin{bmatrix} \check{D}_{22} & -\check{D}_{12} \\ -\check{D}_{21} & \check{D}_{11} \end{bmatrix} \quad (A.49)$$

Expansion of this expression gives

$$A_{11}^{-1} = \frac{M_{11} \tilde{D}_{32} - M_{12} \tilde{D}_{31}}{\tilde{D}_{11} \tilde{D}_{32} - \tilde{D}_{12} \tilde{D}_{31}} \quad (\text{A.50})$$

$$A_{12}^{-1} = \frac{M_{12} \tilde{D}_{11} - M_{11} \tilde{D}_{12}}{\tilde{D}_{11} \tilde{D}_{32} - \tilde{D}_{12} \tilde{D}_{31}} \quad (\text{A.51})$$

$$A_{31}^{-1} = \frac{M_{12} \tilde{D}_{32} - M_{32} \tilde{D}_{31}}{\tilde{D}_{11} \tilde{D}_{32} - \tilde{D}_{12} \tilde{D}_{31}} \quad (\text{A.52})$$

$$A_{32}^{-1} = \frac{M_{32} \tilde{D}_{11} - M_{12} \tilde{D}_{12}}{\tilde{D}_{11} \tilde{D}_{32} - \tilde{D}_{12} \tilde{D}_{31}} \quad (\text{A.53})$$

Setting  $A_{12}^{-1} = -A_{31}^{-1}$  again yields the condition (A.46).

The values for a binary mixture can be obtained by setting the concentration of one species in the ternary mixture equal to zero, say  $C_2$ . In this case  $M_{22} \sim RT/C_2$  as  $C_2 \rightarrow 0$ , and the values of  $M_{11}$  and  $M_{32}$  remain finite.

We obtain then

$$A_{11} \Rightarrow \frac{\tilde{D}_{11}}{M_{11}}, \quad A_{12} \Rightarrow 0, \quad A_{31} \Rightarrow 0, \quad A_{32} \Rightarrow 0, \quad \tilde{D}_{31} \Rightarrow 0. \quad (\text{A.54})$$

The pressure-diffusion coefficients become for a binary mixture

$$D_1^{(p)} \Rightarrow \frac{T \tilde{D}_{11} (R_1 - R_3)}{M_{11}} = \frac{C_1 C_3 (R_1 C_1 + R_3 C_3) (R_1 - R_3) \tilde{D}_{11}}{R_1 R_3} \quad (\text{A.55})$$

$$D_3^{(p)} \Rightarrow 0$$

The inverse coefficient becomes

$$A_{11}^{-1} \Rightarrow \frac{M_{11}}{\tilde{D}_{11}}, \quad A_{12}^{-1} = -A_{31}^{-1} = \frac{M_{12} \tilde{D}_{11} - M_{11} \tilde{D}_{12}}{\tilde{D}_{11} \tilde{D}_{32}} \quad (\text{A.56})$$

$$A_{32}^{-1} \Rightarrow \frac{M_{32}}{\tilde{D}_{32}}$$

Since  $\vec{J}_2$  must vanish we deduce that  $D_3^{(T)}$  vanishes also when  $C_2 \rightarrow 0$ .

Hence for a binary mixture we get the result

$$\vec{J}_1 = -\tilde{D}_{11} \nabla C_1 - \frac{C_1 C_2 (R_1 C_1 + R_2 C_2)(R_1 - R_2)}{R_1 R_2} \tilde{D}_{11} \nabla \ln p - D_1^{(T)} \nabla \ln T, \quad (\text{A.57})$$

$$\vec{J}_2 = 0 \quad (\text{A.58})$$

$$\vec{J}_3 = -\vec{J}_1 \quad (\text{A.59})$$

$$\vec{q} = -k \nabla T + (h_1 - h_3) \vec{J}_1 + \frac{M_{11}}{\tilde{D}_{11}} D_1^{(T)} \vec{J}_1 \quad (\text{A.60})$$

One may verify that these forms are the same as determined by kinetic theory (see Hirschfelder, Curtiss and Bird (1954)). In kinetic theory the coefficients  $\tilde{D}_{11}$ ,  $D_1^{(T)}$ , and  $k$  are determined by the details of the molecular interactions, whereas in the present derivation they are phenomenological coefficients that must be determined empirically.

APPENDIX B

LARGE TIME INVERSION OF CERTAIN LAPLACE

TRANSFORMS

We are concerned here with Laplace transforms of the form

$$\bar{U}(x, s) = \bar{G}(x, s) e^{-x F(s)} \quad (\text{B.1})$$

where  $s$  is the Laplace transform variable and  $\bar{G}(x, s)$  is the transform of  $G(x, t)$ . We assume that  $x$  is positive and that  $F(s)$  is positive when  $s$  is real and positive. The function  $F(s)$  is further restricted such that it is analytic at  $s=0$  and such that  $F(0)=0$ . Such restrictions are associated with wave behaviour. In particular,  $F(s)$  is to be identified with  $\lambda_2(s)$  defined by (4.19).

In the asymptotic limit of large times, we are interested in the corresponding limit  $s \rightarrow 0$  for the Laplace transforms. Thus we write the Taylor series expansion for  $F(s)$  about  $s=0$  as

$$F(s) \sim F'(0)s + \frac{1}{2} F''(0)s^2 + \frac{1}{6} F'''(0)s^3 + \dots \quad (\text{B.2})$$

If only the first term in this expansion is retained, a discontinuous wave front for  $U(x, t)$  is obtained in the inversion of (B.1).

If the next term in (B.2) is retained, no simple and useful means



of inversion is evident. Hence, we wish to devise another expansion for  $F(s)$ , when  $s \rightarrow 0$ , in terms of a function that leads to a relatively simple inversion and in effect retains the first two terms of (B.2).

Consider the following function and its corresponding Taylor series expansion:

$$2ab \left[ \sqrt{s+b^2} - b \right] \sim as - \frac{a}{4b^2} s^2 + \frac{a}{8b^4} s^3 + \dots \quad (\text{B.3})$$

When  $a$  and  $b$  are identified as

$$\begin{aligned} a &\equiv F'(0) \\ b &\equiv \left[ -F'(0)/2F''(0) \right]^{1/2}, \end{aligned} \quad (\text{B.4})$$

then the first two terms of (B.1) and (B.3) are the same. We assume that  $F'(0) > 0$  and  $F''(0) < 0$ , which will be the case in problems associated with dissipative wave behaviour. Taking the difference between (B.2) and (B.3) yields

$$F(s) \sim 2ab \left[ \sqrt{s+b^2} - b \right] + \left[ \frac{1}{6} F'''(0) - \frac{a}{8b^4} \right] s^3 + \dots \quad (\text{B.5})$$

as  $s \rightarrow 0$ . We can now write, for  $s \rightarrow 0$ ,

$$e^{-xF(s)} \sim e^{-2abx \left[ \sqrt{s+b^2} - b \right]} \left[ 1 + \sum_{n=3}^{\infty} K_n(x) s^n \right] \quad (\text{B.6})$$

where

$$K_3(x) \equiv -\frac{x}{6} \left[ F'''(0) - \frac{3a}{4b^2} \right] \quad (\text{B.7})$$

and the remaining  $K_n$ 's can be obtained by laborious algebra.

The inversion of the first term in (B.6) is

$$\mathcal{L}^{-1} \left\{ e^{-\alpha abx [\sqrt{s+b^2} - b]} \right\} = \frac{abx}{\sqrt{\pi}} \frac{e^{-\frac{b^2(t-ax)^2}{t}}}{t^{3/2}} \quad (\text{B.8})$$

By means of the convolution theorem, expression (B.1) with the substitution of (B.6) can be inverted term by term. For the leading term in (B.6), we obtain,

$$U_0(x, t) = \frac{abx}{\sqrt{\pi}} \int_0^t G(x, t-\tau) \frac{e^{-\frac{b^2(\tau-ax)^2}{\tau}}}{\tau^{3/2}} d\tau \quad (\text{B.9})$$

We now observe that  $U_0$  and all its derivatives vanish at  $t = 0$  when  $X > 0$  (since the function (B.8) is exponentially small near  $t \rightarrow 0$  when  $X > 0$ ). Thus the higher-order terms associated with  $S^n$  in (B.6) are related to the corresponding  $n$ th time derivatives of  $U_0$ . The complete asymptotic expansion for large time can thus be written

$$U(x, t) \sim \left[ 1 + \sum_{n=3}^{\infty} K_n(x) \frac{\partial^n}{\partial t^n} \right] U_0(x, t) \quad (\text{B.10})$$

Since the functions  $K_n(x)$  all vanish at  $X=0$ , expression (B.10) is valid at  $X=0$ . The function  $U_0(x, t)$  gives the exact value of  $U(x, t)$  at  $X=0$ .

Consider the example when  $G=1$ , for which  $\bar{G} = 1/5$ .

Evaluation of the integral in (B.9) then gives

$$U_0(x, t) = \frac{1}{2} \left[ \operatorname{erfc} \left\{ \frac{b(ax-t)}{\sqrt{t}} \right\} + e^{4ab^2x} \operatorname{erfc} \left\{ \frac{b(ax+t)}{\sqrt{t}} \right\} \right] \quad (\text{B.11})$$

When  $G = \delta(t)$  and  $\bar{G} = 1$ , we have

$$U_0(x, t) = \frac{abx}{\sqrt{\pi}} \frac{e^{-\frac{b^2(t-ax)^2}{t}}}{t^{3/2}} \quad (\text{B.12})$$

It may be suitable in some situations to expand the function  $\bar{G}(x, s)$  in powers of  $s$ , isolating singularities that occur at  $s = 0$ . A result similar in form to (B.10) can then be found.