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Since the early 1970's activation energy asymptotics (AEA) has dominated the analysis of combustion. In more recent years attempts have been made to use this tool for the study of flame structure with multistep kinetics. In certain instances the AEA approach has led to solutions that do not resemble the numerical solutions of the full equations, as in the ozone decomposition flame for example, or physically unrealistic assumptions are made to force the solution to look realistic as in the analysis of stretch resistant flames. These difficulties have been overcome through the use of large heat release asymptotics (LHRA). The developement and implementation of this technique is outlined in this report through the examination of the far field structure of a premixed flame with multistep kinetics, the finding of a new similarity solution for reacting gas flow, and the analysis of a strained flame with multistep kinetics.

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PREFACE

This final report was submitted by the University of Florida, under Contract No. AFOSR-87-0236. The program was managed by Dr. Arje Nachman of AFOSR. The principle investigator was Dr. David W. Mikolaitis of the Department of Aerospace Engineering, Mechanics, and Engineering Science at the University of Florida. This research was initiated in June, 1987 and completed in June, 1988. This report was written by Dr. David W. Mikolaitis.

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INTRODUCTION

The main thrust of mathematical analysis of deflagration and detonation waves since the early 1970's has been through the application of activation energy asymptotics (AEA) as in Buckmaster and Ludford (1982). While this approach is of great utility in many problems of practical interest, there are also many cases where the activation energy cannot be taken as large, such as in hydrogen oxidation. There is little doubt that hydrogen will be an important fuel in the coming decades since the need for energy sources with high specific energy (automobiles, aircraft, Space Shuttle, etc) will be with us for the foreseeable future and concerns, both real and imagined, over the release of carbon dioxide into the environment are mounting.

With these concerns in mind, mathematical methods for the study of combustion phenomena needed to be developed through the application of large heat release asymptotics (LHRA). Previous work in this area for deflagration waves is scant (Mikolaitis, 1986a, 1986b, 1987a) although similar ideas have been used in the analysis of well stirred reactors (Gray, 1973). In Mikolaitis (1986a), the structure of the adiabatic, plane deflagration wave with one step, irreversible kinetics is studied under the limit of large heat release. In Mikolaitis (1986b), a similar analysis is undertaken for the two-step Zeldovich-Liñán model that includes a chain branching mechanism and a termination step. The motivation of this work was to show that the usual AEA analyses of this problem do not result in a realistic flame structure over the entire range of flame temperatures but LHRA analyses do.

THE ELEMENTS OF LARGE HEAT RELEASE ASYMPTOTICS

Rates of reaction generally follow an Arrhenius rate of the form

$$\text{rate} = B\ [F]^a[O]^b T^n \exp(-E_a/RT)$$

where [F] and [O] are the concentrations of species F and O, T is the absolute temperature, R is the universal gas constant, B is the pre-exponential constant, a and b are the stoichiometric integers (these need not be integers if this rate expression is a model for a more complicated reaction mechanism), n is the algebraic temperature dependence, and E_a is the activation energy. E_a/R has units of temperature and is called the activation temperature.

In AEA it is assumed that E_a/R is very much greater than the temperature of the reacting gases everywhere. A consequence of this assumption is that reaction is confined to a thin sheet with frozen reaction on one side and equilibrium on the other. The diffusion of heat and mass, on the other hand, take place on a much longer length scale.

In LHRA, E_a/R is taken to be of the same order of magnitude as the flame temperature but large compared to the reactant supply temperature. The resulting flame structure in this limit has reaction distributed on the same length scale as the diffusion of mass and heat and so the reaction zone and preheat zone of the flame are of similar thicknesses.

As a concrete example, let us analyze the structure of the downstream far-field of an adiabatic, laminar premixed flame.

The adiabatic, laminar premixed flame problem involves the search for a steady solution to a set of nonlinear ordinary differential equations on a doubly infinite domain. Cool, fresh reactants are supplied far upstream of the flame and hot, burned gases in equilibrium exist far behind the flame. The mass flux of material normal to the flame is a parameter in the set of differential equations and is to be determined as part of the solution. Determining the mass flux is usually the goal of the analysis. Of course, finite differencing for the numerical solution of the governing equations subject to boundary

conditions on a doubly infinite domain is not a practical problem and so the computational domain must be truncated.

The typical computational approaches for the cold boundary are to assume a zero reaction rate between $x=-\infty$ and some position $x=a$ and integrate the resulting equations to arrive at boundary conditions at $x=a$ or simply to transfer the cold remote conditions directly to $x=a$. Both of these approaches neglect the "cold boundary difficulty". Since the incoming stream of reactants is not in equilibrium (otherwise it would have no chemical enthalpy that could be turned into heat), the incoming stream must have a positive rate of reaction and so the conditions at infinity are not a solution to the field equations (the reaction term is positive but the convective and diffusive terms must be zero and so cannot balance the reaction term). In practice a steady solution appears to exist due to the fact that real flames only propagate finite distances and the rate of reaction in reactant stream is very small. This allows the flame to reach the combustible mixture long before any appreciable reaction takes place in the fresh mixture at the cool reactant temperature. One of the triumphs of AEA was that it allowed a rational analysis of the steady flame problem without introducing in an ad hoc manner any extraneous term in the reaction rate expression. One simply realizes that the "steady" solution is the leading order solution to an intrinsically unsteady problem. Here we have generalized this idea through LHRA. It is not necessary that the activation temperature be considered as large compared to the flame temperature but only that the activation temperature is large compared to the cool reactant temperature. When viewed in this way, AEA is seen to be a limiting case of the more general treatment through LHRA.

For the hot boundary it is typical to specify equilibrium conditions at some position $x=a+L$ where L is "sufficiently" large. The sufficiency is usually tested by increasing L and comparing the resulting value of the steady-state mass flux with the previously calculated value. It is typical to consider a 2%

change as small.

Here we will show how an analysis of the downstream far-field of a laminar adiabatic premixed flame can be accomplished through a series of simple example problems that are of interest in relation to several large activation energy analyses that have appeared in the recent literature. The results of an analysis such as this can be used to apply boundary conditions a finite distance behind the flame consistent with the far-field structure. This should ameliorate any errors introduced through the truncation of the computational domain. It may also make it possible to use a smaller computational domain in practice since the boundary conditions derived from this analysis have the correct approach to equilibrium built into them and so this fairly slow process need not be reproduced in the finite difference scheme.

There are no conceptual differences between the examples to be investigated here and examples with complete chemical kinetics and sophisticated multi-component transport models.

A FOUR-STEP MODEL

Changes in kinetic mechanism with flame temperature have been invoked to explain certain phenomena peculiar to flame propagation through very lean hydrogen mixtures (Peters and Smooke, 1985). The Peters-Smooke four-step model in essence is a chain branching mechanism, a product formation reaction, and a reaction that consumes chain carriers and produces an inert intermediate (chain termination). At sufficiently low temperatures the chain termination mechanism dominates the chain branching mechanism and effectively terminates the reaction by eliminating all the active radicals. Peters and Smooke (1985) analyzed the response of a premixed flame with this kinetic mechanism to small aerodynamic straining (weak flame stretch) under a fast recombination/large activation energy limit. Under

the influence of weak flame stretch, such premixed flames with Lewis numbers less than one (such as lean hydrogen/air mixtures) will experience a rise in temperature above the adiabatic flame temperature. This then was used to explain how hydrogen/air mixtures nominally below the lean limit can support cellular flames and why the troughs of such flames, where the flame experiences positive flame stretch, are much brighter than the crests (which may be extinguished) where the flame is compressed and hence cooled.

Although this explanation is very appealing (and probably correct for the most part) it leaves some questions unanswered. First of all, an O(1) increase in flame temperature above the adiabatic value is required to move the flame temperature of the very lean hydrogen-air mixtures above the transition temperature. This requires O(1) flame stretch. The analysis of Peters and Smooke only allowed weak flame stretch. In addition, HO_2 is <u>not</u> inert. There are reaction paths, albeit slow ones, through which HO_2 can react to form more active radicals through an alternate branching cycle involving the formation of hydrogen peroxide, H_2O_2. Previous analytical work in detonation wave structure (Mikolaitis, 1987b) has shown that the existence of this alternate branching cycle has an O(1) effect on the length of the induction zone of even stoichiometric hydrogen-air detonation waves. It is well known that lean premixed hydrogen-air flames show appreciable levels of hydrogen peroxide. It is also well known that appreciable changes in flame speed occur if HO_2 chemistry is ignored. For these reasons it is very likely that HO_2 chemistry plays a major role in low temperature hydrogen-air premixed flames. Peters and Smooke's treatment assumes that the slow chemistry of this species is infinitely so.

As a start of a more general analysis of this problem, we will first introduce a four-step reaction scheme that has both a high temperature and low temperature mechanism. Secondly we will analyze the far field flame structure that results from this mechanism in a general context that allows O(1) activation

energies (as opposed to restricting the validity of the analysis to the large activation energy limit).

REACTION MODELING

As is well known from reaction vessels studies, the way in which oxygen reacts with hydrogen at low temperatures is very different from the way they react with each other at high temperatures. The source of this change in kinetic mechanism is the competition between the reactions $H + O_2 \rightarrow O + OH$ and $H + O_2 + M \rightarrow HO_2 + M$ where M is a third body. The products of the first reaction readily react with H_2 to form additional radicals while HO_2 reacts with H_2 to form H_2O_2 (hydrogen peroxide). The peroxide intermediate dissociates into two hydroxyl radicals through a relatively slow, large activation temperature reaction. These OH radicals then quickly react with H_2 to form additional radicals.

Here we will study a simplified kinetic model that has the following features:

1) a chain branching mechanism that dominates at high temperatures,

2) a chain branching mechanism that dominates at low temperatures,

and

3) a product formation/termination reaction.

This can be most easily accomplished through the four-step mechanism

$$A + X = X + X \tag{1}$$

$$X + X = P + P \tag{2}$$

$$A + X = Y + Y \tag{3}$$

$$X + Y = X + X. \tag{4}$$

A represents the major reactants, X represents the highly

reactive radicals, Y represents the relatively inert intermediates and P represents the final product. Forward reaction (1) is a chain branching reaction, (2) is the product formation/termination step, (3) competes with (1), and (3) and (4) taken together ((3) + 2 x (4)) is another chain branching mechanism. The set of forward reactions (1-2) forms the Zeldovich-Liñán mechanism that has been extensively studied in recent years (Liñán, 1971, Seshadri and Peters, 1983, Tam and Ludford, 1984, 1985, Joulin, et al, 1985, Mikolaitis, 1986b).

Numerical subscripts will refer to the reaction numbers 1 to 4. Positive subscripts will refer to the forward reactions and negative subscripts will refer to the reverse reactions. All reaction rates will be assumed to be proportional to the mass fraction of each reactant and have a general temperature dependence. For example, the rate of reaction for the reverse reaction (1) is $X^2 f_{-1}(T)$. Of course, Arrhenius reaction rates are a special case of this more general form.

GOVERNING EQUATIONS

Under the assumption of calorifically perfect gases with constant transport properties and also assuming low Mach numbers, the non-dimensional governing equations describing a one-dimensional reacting front with the aforementioned four-step chemistry are

$$MT' = T'' + q_1(AXf_1 - X^2 f_{-1}) + q_2(X^2 f_2 - P^2 f_{-2}) + q_3(AXf_3 - Y^2 f_{-3}) + q_4(XYf_4 - X^2 f_{-4}) \tag{5}$$

$$MA' = \frac{1}{L_A} A'' - (AXf_1 - X^2 f_{-1}) - (AXf_3 - Y^2 f_{-3}) \tag{6}$$

$$MX' = \frac{1}{L_X} X'' + (AXf_1 - X^2 f_{-1}) - 2(X^2 f_2 - P^2 f_{-2}) - (AXf_3 - Y^2 f_{-3}) + (XYf4 - X^2 f_{-4}) \tag{7}$$

$$MY' = \frac{1}{L_Y} Y'' + 2(AXf_3 - Y^2 f_{-3}) - (XYf_4 - X^2 f_{-4}) \tag{8}$$

$$P = 1 - A - X - Y. \tag{9}$$

M is the mass flux normal to the flame (constant); T is the temperature; A, X, Y and P are the mass fractions of species A, X, Y and P respectively; L_A, L_X and L_Y are the appropriate Lewis numbers; and the q's are the heat releases. Since the heat release for species A being converted into species B must be independent of reaction path, we have the additional relationship

$$q_4 = (q_1 - q_3)/2. \tag{10}$$

The boundary conditions far behind the flame are that the mixture is in equilibrium.

THE EQUILIBRIUM STATE

For a given final temperature, T_b, where the subscript b denotes the burned state, the equilibrium state is very easily ascertained in closed form. If we define

$$C = \frac{-f_4 + \sqrt{f_4 + 8(f_{-4} + \frac{2f_{-1}f_3}{f_1+f_3})(\frac{f_1 f_{-3}}{f_1+f_3})}}{\frac{4f_1 f_{-3}}{f_1+f_3}} \tag{11}$$

and

$$K = (f_{-1} + \alpha^2 f_{-3})/(f_1 + f_3) \tag{12}$$

where the reaction rate functions are evaluated at the burned temperature, T_b, then

$$A_b = K X_b, \tag{13}$$

$$Y_b = C\,X_b, \tag{14}$$

and X_b satisfies the quadratic

$$X_b^2(-Kf_1+f_{-1}+2f_2-2(1+C+K)^2f_{-2}+Kf_3-C^2f_{-3}-Cf_4+f_{-4}) + 4X_b(1+C+K)f_{-2} -2f_{-2} = 0. \tag{15}$$

The state of the burned gases is linked to the state of the fresh reactants through the total enthalpy. Multiplying (6) by $(q_1+q_2/2)$, (7) by $q_2/2$, and (8) by $(q_1+qa_2-q_3)/2$ and adding these results to (5) yields after integration and the application of boundary conditions

$$T_f + (q_1+q_2/2)A_f + q_2X_f/2 + (q_1+q_2-q_3)Y_f/2 = \tag{16}$$

$$T_b + (q_1+q_2/2)A_b + q_2X_b/2 + (q_1+q_2-q_3)Y_b/2$$

where the subscript f denotes the remote, fresh state. Specification of the cool, fresh reactant state fixes the constant in (16) and hence substitution of (13-15) into (16) yields a single equation for the burned gas temperature.

PHASE SPACE EQUATIONS AND PERTURBATIONS TO EQUILIBRIUM

The system of equations (5-8) are autonomous and hence the independent variable x can be replaced with one of the dependent variables. In most cases T can be used without difficulty. The system is thereby reduced in order by one and the domain of the adiabatic plane flame problem goes from being doubly infinite ($-\infty<x<+\infty$) to finite ($T_f<T<T_b$ where T_f is the temperature of the cool, fresh reactants). Letting $z = T'$, the governing equations become

$$Mz = z\frac{dz}{dT} + q_1(AXf_1 - X^2 f_{-1}) + q_2(X^2 f_2 - P^2 f_{-2})$$

$$+ q_3(AXf_3 - Y^2 f_{-3}) + q_4(XYf_4 - X^2 f_{-4}) \tag{17}$$

$$Mz\frac{dA}{dT} = \frac{1}{L_A} z \frac{d}{dT}\left(z\frac{dA}{dT}\right) - (AXf_1 - X^2 f_{-1}) - (AXf3 - Y^2 f_{-3}) \tag{18}$$

$$Mz\frac{dX}{dT} = \frac{1}{L_X} z \frac{d}{dT}\left(z\frac{dX}{dT}\right) + (AXf_1 - X^2 f_{-1}) - 2(X^2 f_2 - P^2 f_{-2})$$

$$- (AXf_3 - Y^2 f_{-3}) + (XYf_4 - X^2 f_{-4}) \tag{19}$$

$$Mz\frac{dY}{dT} = \frac{1}{L_Y} z \frac{d}{dT}\left(z\frac{dY}{dT}\right) + 2(AXf_3 - Y^2 f_{-3}) - (XYf_4 - X^2 f_{-4}) \tag{20}$$

along with (9). One of these equations may be replaced by an enthalpy relation. When $T=T_b$, equilibrium holds so that

$$A(T_b) = A_b,\ X(T_b) = X_b,\ Y(T_b) = Y_b, \tag{21}$$

and

$$z(T_b) = 0. \tag{22}$$

The price that one pays when converting a problem on an infinite domain to one on a finite domain is that now one has a boundary value problem that is singular at both endpoints. Here we will be numerically integrating the governing equations (17-20) from one end point toward the other. It is therefore necessary to analyze the local structure of the singularity in order to specify proper initial conditions slightly away from the singular point.

Perturbations to the hot singular point can be analyzed through the expansions

$$z=\epsilon\zeta,\ A=A_b+\epsilon\delta,\ X=X_b+\epsilon\chi,\ Y=Y_b+\epsilon\psi,\ T=T_b+\epsilon\tau,\ \epsilon<<1. \tag{23}$$

and the boundary conditions (21-22) become

$$\zeta(0)= (0)=\chi(0)=\psi(0)=0. \tag{24}$$

The non-linear limit equations resulting from the expansions (23) are easily solved subject to the initial conditions (24). The system admits a solution of the form

$$\delta = a\tau, \quad \psi = b\tau, \quad \chi = c\tau, \quad \zeta = g\tau \tag{25}$$

that satisfy (24) if a, b, c and g satisfy the algebraic relationships

$$Mg = g^2 + q_1A_1 + q_2A_2 + q_3A_3 + q_4A_4 \tag{26}$$

$$Mga = \frac{1}{L_A} g^2a - A_1 - A_3 \tag{27}$$

$$Mgb = \frac{1}{L_Y} g^2b + 2A3 - A_4 \tag{28}$$

$$Mgc = \frac{1}{L_X} g^2c + A_1 - 2A_2 - A_3 + A_4 \tag{29}$$

where

$$A_1 = aX_bf_1 + A_bcf_1 + A_bX_bf_1' - 2X_bcf_{-1} - X_b^2f_{-1}' \tag{30}$$

$$A_2 = 2X_bcf_2 + X_b^2f_2' - (1-A_b-X_b-Y_b)^2f_{-2}' + 2(1-A_b-X_b-Y_b)(a+b+c)f_{-2} \tag{31}$$

$$A_3 = A_bcf_3 + X_baf_3 + A_bX_bf_3' - 2Y_bbf_{-3} - Y_b^2f_{-3}' \tag{32}$$

$$A_4 = Y_bcf_4 + X_bbf_4 + X_bY_bf_4' - 2X_bcf_{-4} - X_b^2f_{-4}'. \tag{33}$$

The temperature dependency functions (f_i functions) and their derivatives are to be evaluated at the burned gas temperature T_b.

The derivative of z with respect to T is identical with T"/T'. Since T approaches a constant, T_b, as x goes to infinity, T"/T' is negative for large values of x. This implies that dz/dT must be negative in the neighborhood of T_b and so g cannot be positive.

A solution to this system of algebraic equations can be

found with $g=0$ and a, b and c satisfying a set of three linear algebraic equations whose solution in closed form is easily accomplished. The implication of $g=0$ in the neighborhood of $T=T_b$ is that the conditions of the burned gas far behind the flame is dominated solely by chemical reaction with convection and conduction/diffusion playing no role. This spatially homogeneous solution also corresponds to the final approach to equilibrium of a quiescent gas in an adiabatic enclosure. Of the multiple solutions to the set (26-29), this is <u>not</u> the appropriate choice as can be easily determined.

Letting $\alpha=q_1+q_2/2$, $\beta=q_2/2$, $\gamma=(q_1+q_2-q_3)/2$, it is easily shown that

$$M(T + \alpha A + \beta X + \gamma Y) = z(1 + \frac{\alpha}{L_A}\frac{dA}{dT} + \frac{\beta}{L_X}\frac{dX}{dT} + \frac{\gamma}{L_Y}\frac{dY}{dT}) + C \qquad (34)$$

is true globally where C is a constant that can be evaluated at either the hot or cold singular point. If (34) is differentiated with respect to T and evaluated at $T=T_b$ with the further restriction that $dz/dT = 0$ at that point (so that $g=0$), then

$$1 + \alpha a + \beta c + \gamma b = 0. \qquad (35)$$

This constraint is inconsistent with the solution to the three linear algebraic equations for a, b and c, i.e. (27-29) with $g=0$, unless the three Lewis numbers are all exactly one. The case where all the Lewis numbers are unity will be discussed later. Therefore, although there is a solution for $g=0$, that solution violates a global constraint and hence is of no interest in this problem. We shall now consider only solutions with g strictly less than zero.

Solutions to (26-29) with $g<0$ can be found numerically. The computational difficulty is significantly reduced through the derivation of the auxiliary equation

$$g = \frac{M(1 + \alpha a + \beta c + \gamma b)}{1+(\alpha a/L_A)+(\beta c/L_X)+(\gamma b/L_Y)} \qquad (36)$$

to be used in place of one of the original equations. Through the use of this equation not only is the unwanted root with g=0 avoided, the permissible solution space in the abc space is easily located between the planes where the numerator and the denominator of (36) are zero. Since in practice the Lewis numbers L_A, L_X and L_Y can be quite close to one, it is clear that the permissible solution space can become two very narrow wedges. In such situations, knowledge of these bounds on the solution space is critical in determining a suitable "first guess" for numerical root finding on this system of non-linear algebraic equations.

THE SPECIAL CASE OF UNIT LEWIS NUMBERS

When all the Lewis numbers are identically one, there is a further reduction in the complexity of the problem. Equation (34) can be integrated once again to give

$$T + \alpha A + \beta X + \gamma Y = \text{constant} \tag{37}$$

so that

$$1 + \alpha \frac{dA}{dT} + \beta \frac{dX}{dT} + \gamma \frac{dY}{dT} = 0. \tag{38}$$

We therefore now know one of the a,b,c's explicitly in terms of the other two. Furthermore, g can now be found in terms of two

of the a,b,c's through the quadratic solution of (26), that is

$$g = (M - \sqrt{M^2-4(\Sigma A_i q_i)})/2, \tag{39}$$

where the negative root is taken as the only possible way to generate a negative value of g.

THE REVERSIBLE ZELDOVICH-LINAN MECHANISM

A subset of the reaction mechanism (1-4) consisting of the forward reactions 1 and 2 has received considerable attention through the years (Zeldovich, 1948, Liñán, 1971, Seshadri and Peters, 1983, Tam and Ludford, 1984, 1985, Joulin et al, 1985, Mikolaitis, 1986b). If the alternate branching mechanism is very slow compared to the main chain branching mechanism and it is found that there is negligible amounts of Y at equilibrium, then the low temperature mechanism (3-4) can be ignored. This is the typical case when the flame temperature is high. Here we will analyze the two-step mechanism (1-2) where each reaction is reversible in order to take into account equilibrium dissociation of the product. This is not an element of the earlier analyses of this mechanism.

The equilibrium state as a function of burned gas temperature is easily determined to be

$$X_b = \frac{1}{1+f_{-1}/f_1+\sqrt{f_2/f_{-2}}}, \quad A_b = f_{-1}X/f_1, \quad P_b = 1-A_b-X_b \tag{40}$$

where the temperature dependency functions, f_i, are evaluated at the burned gas temperature T_b. Expanding A, X and T in the neighborhood of the equilibrium point through

$$A = A_b + \epsilon\delta, \quad X = X_b + \epsilon\chi, \quad T = T_b + \epsilon\tau, \quad z = \epsilon\zeta \tag{41}$$

leads to a set of nonlinear ordinary differential equations

subject to the initial conditions

$$\delta(\tau=0)=\chi(\tau=0)=\zeta(\tau=0)=0. \tag{42}$$

This set of nonlinear differential equations admit solutions of the form

$$\delta=a\tau,\ \chi=c\tau,\ \zeta=g\tau \tag{43}$$

if a, c and g satisfy the algebraic equations

$$Mg = g^2 + q_1B_1 + q_2B_2 \tag{44}$$

$$Mga = \frac{1}{L_A} g^2a - B_1 \tag{45}$$

$$Mgc = \frac{1}{L_X} g^2c + B_1 - 2\ B_2 \tag{46}$$

where

$$B_1 = aX_bf_1 + A_bcf_1 + A_bX_bf_1' - 2X_bcf_{-1} - X_b^2f_{-1}' \tag{47}$$

and

$$B_2 = X_bcf_2 + X_b^2f_2' + 2(1-A_b-X_b)(a+c)f_{-2} -(1-A_b-X_b)^2f_{-2}'. \tag{48}$$

These solutions also satisfy the initial conditions (42). As before, there is a solution to this set of equations with g=0, but again this solution is not appropriate. In order to avoid this unwanted solution if numerical root finding is used it is advantageous to rearrange (44-46) to arrive at

$$g = \frac{M(1+\alpha a+\beta c)}{1+\alpha a/L_A+\beta c/L_X} \tag{49}$$

provided that not both L_A and L_X are unity.

If both Lewis numbers are unity then an exact solution with physically sensible behavior is easily achieved. In that case a

and c are related through

$$1 + \alpha a + \beta c = 0. \tag{50}$$

(45) is then divided by a and subtracted from (44). Elimination of c from the resultant yields a quadratic in a.

CONCLUDING REMARKS ON THE EXAMPLE PROBLEM

The approach to equilibrium behind the adiabatic premixed flame is a very slow process that typically takes place on a long length scale compared to the primary reaction zone thickness and the heat conduction - major species diffusion length scale. Here we have analyzed the structure of the approach to equilibrium behind a premixed flame front for a four step reaction model. The simultaneous non-linear ordinary differential equations that describe the process can be solved exactly up to a set of constant coefficients. The required coefficients are found through a set of simultaneous algebraic equations that can be solved numerically.

The mathematical algorithm used in this example problem can also be used in the general context of a complete chemical kinetic mechanism with variable transport coefficients. We are currently investigating the ozone decomposition flame as an example problem. Through such a solution the boundary conditions an infinite distance behind the reacting front can be brought to a finite distance behind the reacting front without a substantial loss of accuracy. It is also possible to reduce the computational domain for the calculation of an adiabatic plane premixed flame structure significantly because the long approach to equilibrium will be known analytically and need no longer be resolved numerically.

A NEW SIMILARITY SOLUTION FOR REACTING GAS FLOWS

In the AEA analysis of premixed flames the analog to the stagnation point flow similarity solution is very similar to the non-reacting stagnation point flow in that the gas velocities at infinity are singular. Since this is the case, the applicability of the analysis is restricted to the boundary layer applications where the flame is restricted to be close to the stagnation plane even though the solution is a solution of the full Navier-Stokes equations.

Under the limit of LHRA, this is no longer the case. Solutions for reacting opposed flow are found where the velocity at infinity is finite and uniform without slip as in boundary conditions for flow exiting a porous plug. This means that the realistic boundary conditions are met for the full problem and restriction to a boundary layer solution is not necessary. A copy of the page proofs of an article on this solution is included as Appendix A.

Why is the character of the solution different in the limit of large heat release? The essential difference between the two solutions is that in the AEA stagnation point flow type solution there is a quadratic variation in pressure transverse to the flame whereas in the LHRA solution the transverse pressure gradient is required to be zero to leading order. There is a mathematical argument to show that this must be true, but a non-rigorous physical argument can be made that is more revealing.

In the study of gaseous bubbles rising through liquids, where there is a great difference between the density of the gaseous phase and the liquid phase, the density ratio between the liquid and gas phases can be approximated by infinity (i.e., zero density for the gas phase to leading order). Under these circumstances free streamline theory can be applied and in this theory the material surface separating the high momentum outer flow of the liquid phase from the stagnant (to leading order) wake fluid in the gaseous phase is a surface of constant

pressure. In the LHRA analysis of opposed flow we have a very similar situation where the flame plays a role analogous to that played by the material surface in free streamline theory. It should therefore not be surprising that LHRA predicts zero transverse pressure gradient and low momentum far behind the flame.

The LHRA analysis also predicts some very interesting behavior that cannot be predicted through AEA. It is well known that when premixed flames with Lewis numbers less than one are positively stretch, the flame temperature rises. If adiabatic conditions are enforced far behind the flame, the AEA analysis of such a stretched premixed flame would never predict extinction and the flame temperature would continuously rise with increasing stretch. If conductive heat loss to the gases far behind the flame is allowed by specifying a low temperature for the remote, burned products, then as the flame stretch is increased the flame temperature will eventually fall (but only after the flame has retreated far into the opposed flow) and the flame structure has become quite diffuse. This mathematical behavior has been interpreted as extinction even though mathematical flame structures still exist. In LHRA, a new extinction behavior is found that is very easy to understand and remarkable in that it at first seems counter-intuitive: Flames can extinguish by becoming too hot! The physics of this mechanism is very simple. In Arrhenius kinetics the rate of reaction has a temperature dependence that goes monotonically from 0 to a positive constant as the temperature goes from zero to infinity and the approach to zero is through exponentially small functions. The rate of reaction is proportional to this quantity times the concentration of the reactants. These concentration go monotonically from infinity to zero as the temperature goes from 0 to infinity and the approach to infinite concentrations is through algebraically large functions. This means that the rate of reaction is zero for both 0 and infinite temperature and finite and positive in between. The rate of reaction therefore has a maximum at some

well defined temperature. The LHRA analysis of the far-field of stretched premixed flames shows that a necessary condition for flames to exist is that the flame temperature is at or below the temperature that gives the maximum reaction rate. Since positive flame stretch increases the flame temperature in flames with Lewis numbers less than one, an upper bound on the flame stretch that such a flame can endure is found.

It should be pointed out that the similarity solution given in Appendix A is a much closer analog to experiment than the stagnation point flow solutions whenever the flame is away from the stagnation plane.

CONTINUING WORK IN LHRA

In the short term, work is continuing in LHRA along two fronts: the analysis of ozone decomposition flames and the generation of other premixed flame structures with multi-step kinetics. The ozone flame is a particularly attractive example problem because it has been studied through conventional numerical approaches (Heimerl and Coffee, 1980) and through conventional AEA methods (Rogg and Wichman, 1985, amoung others). The results of this analysis (undertaken as part of a Master's program by a graduate student at the University of Florida, Department of Aerospace Engineering, Mechanics and Engineering Science) should be more accurate than both the numerical solutions where 2% convergence was deemed adequate and the AEA solutions where reaction is mathematically restricted to a much thinner region than is seen in practice.

In the long term, it is hoped that this research will result in faster computing methods for the prediction of flame structures for both stretched and unstretched premixed flames through the generalization to complete chemical kineteics of the mathematical results generated so far. It is envisioned that this process can be completely automated so that the user need

simply enter the kinetic scheme that is to be used and the program will automatically construct the far-field solution and so forth.

Another application of LHRA is in the study of diffusion flames. This will require a different methodology because the temperature is not monotonic through the flame structure. There are other variables that are, however, and so this is not an insurmountable problem.

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APPENDIX A

Page proofs of a paper entitled

"On the Abrupt Extinction of Premixed Flames with Lewis Numbers Less Than One"

by

David W. Mikolaitis

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On the Abrupt Extinction of Premixed Flames with Lewis Numbers Less Than One

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Abstract—Here we have analyzed the governing equations of reacting low Mach number flow for plane premixed flame structures in non-uniform flow fields given that the activation temperature of the mixture is large compared to the temperature of the remote reactants. An extinction mechanism is uncovered for flames with Lewis numbers less than one that cannot be found through the use of activation energy asymptotics, a limit where the activation temperature of the mixture is large compared to the burned gas temperature.

INTRODUCTION

A central problem in combustion theory is to understand the influence of non-uniform flows on burning rate. A particularly simple model problem that has been extensively studied through the use of activation energy asymptotics (AEA) is the premixed flame in an opposed flow with $A \rightarrow B$ irreversible kinetics. Analysis of this problem have been performed under the constant density approximation (Buckmaster, 1979, and Buckmaster and Mikolaitis, 1982) and with full fluid mechanical coupling under a boundary layer approximation (Libby and Williams, 1982, 1983, 1984, and Libby, Liñán, and Williams, 1983). None of these studies have revealed an abrupt extinction mechanism for adiabatic premixed flames with Lewis numbers sufficiently less than one.

Here we will perform an analysis of the premixed flame in an opposed flow without making a boundary layer approximation or assuming that the activation energy is large. All we will assume is that the activation temperature is large compared to the temperature of the cool remote reactants and that the burned gas temperature is on the order of magnitude of the activation temperature. In this way the concept of an adiabatic flame speed is retained by making the reaction rate of the cool reactants exponentially small compared to the reaction rate in the flame itself. Reaction will no longer confined to a thin sheet, however. Instead, reaction will be distributed on a length scale comparable to the length scale of the temperature field. This has proven to be a more realistic flame structure for relatively hot ozone flames (Mikolaitis, 1987) and in all likelihood will apply to many other situations.

This is also in accord with the results of Coffee, Kotlar, and Miller (1984) who have studied the overall reaction concept as applied to 50% ozone–50% diatomic oxygen, 40% hydrogen–60% air, and stoichiometric methane–air premixed flames. At nominal laboratory conditions for the state of the cool reactants (300 K and 1 atmosphere), the global activation temperatures are 3974 K, 3271, and 15 680 K with burned gas temperatures of 1943 K, 2215 K, and 2232 K, respectively. These give burned gas temperature to activation temperature ratios of 0.489, 0.677, and 0.143 for 50% ozone–50% air, 40% hydrogen–60% air, and stoichiometric methane–air premixed flames. Such numbers will be considered as $O(1)$. The corresponding ratios of cool reactant temperatures to the activation temperature are 0.0755, 0.0917, and 0.0191. These will be considered as small.

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We will non-dimensionalize our governing equations in the same manner as in Mikolaitis (1987) where a similar problem was analyzed under the restriction of unit Lewis number. As Lewis number effects have proven to be very important in the AFEA analyses of flames with flow non-uniformities, it would seem likely that the same would apply here. Since we are interested in low speed deflagration waves, a low Mach number approximation is appropriate so that the resulting steady two dimensional governing equations are:

$$\partial(\varrho u)/\partial x + \partial(\varrho v)/\partial y = 0 \tag{1}$$

$$\partial(\varrho u T)/\partial x + \partial(\varrho v T)/\partial y = \nabla^2 T + Q\varrho T^m Y \exp(-1/T) \tag{2}$$

$$\partial(\varrho u Y)/\partial x + \partial(\varrho v Y)/\partial y = 1/L\, \nabla^2 Y - \varrho T^m Y \exp(-1/T) \tag{3}$$

$$\varrho u \partial u/\partial x + \varrho v \partial u/\partial y = -\partial p/\partial x + P(\nabla^2 u + (\partial(\partial u/\partial x + \partial v/\partial y)/\partial x)/3) \tag{4}$$

$$\varrho u \partial v/\partial x + \varrho v \partial v/\partial y = -\partial p/\partial y + P(\nabla^2 v + (\partial(\partial u/\partial x + \partial v/\partial y)/\partial y)/3) \tag{5}$$

$$\varrho = 1/T \tag{6}$$

for continuity, energy, species conservation, x and y momentum, and equation of state. We have assumed in the derivation of these equations calorifically perfect gases of equal specific heats and constant transport properties. The parameters L and P are the Lewis number and the Prandtl number respectively. T is the temperature non-dimensionalized with respect to the activation temperature of the reaction. u and v are the x and y components of velocity. p is the non-dimensionalized variation in pressure about the ambient combustion pressure, and Y is the mass fraction of reactants. Lengths have been scaled so that the coefficient of the Laplacian of T is unity and velocities have been scaled so that the coefficient of the reaction term is unity. Q is the non-dimensional heat release. The details of the non-dimensionalization can be found in Mikolaitis (1987).

Plane flames where the x-axis is normal to the flame and the y-axis is parallel to the flame (see Figure 1) will require that

$$T = T(x), \quad Y = Y(x), \quad u = u(x). \tag{7}$$

The equation of state immediately gives $\varrho = \varrho(x)$ so that we can define

$$M \equiv \varrho(x)\, u(x) = M(x). \tag{8}$$

Continuity now requires that

$$v = -y\, T\, dM/dx. \tag{9}$$

This x momentum equation (4) now shows that $\partial p/\partial x$ is a function of x only. This then implies that

$$\partial^2 p/\partial x \partial y = 0. \tag{10}$$

Substituting the right hand side of (9) for v and M for ϱu in the y momentum Eq. (5) gives

$$\partial p/\partial y = -y(P d^2(T dM/dx)/dx^2 - M d(T dM/dx)/dx + T(dM/dx)^2). \tag{11}$$

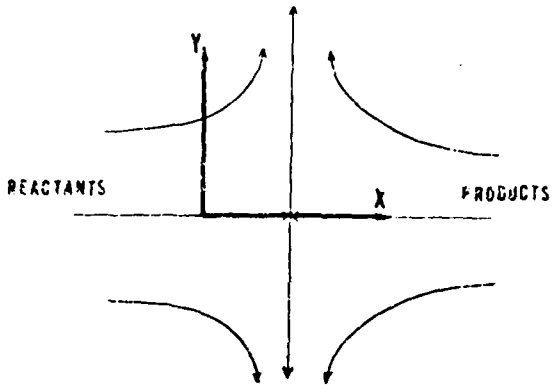

FIGURE 1 Sketch of the flow field and coordinate system.

Applying the condition (10) results in

$$Pd^2(TdM/dx)/dx^2 - Md(TdM/dx)\,dx + T(dM/dx)^2 = \text{const} \qquad (12)$$

so in general one can expect quadratic variations in pressure in the y direction (transverse to the flame) for plane flames as long as the constant in (12) is non-zero. Later we will demonstrate that this quadratic variation is inconsistent with the large heat release limit so that the constant must be zero.

The energy and species conservation equations (2–3) become

$$M\,dT/dx = d^2T/dx^2 + QT^{n-1}\,Y\exp(-1/T) \qquad (13)$$

$$M\,dY/dx = (1/L)d^2Y/dx^2 - T^{n-1}\,Y\exp(-1/T). \qquad (14)$$

We now have a system of 3 non-linear ordinary differential equations to solve given by (12–14).

LARGE HEAT RELEASE ASYMPTOTICS

The central notion of the approximation scheme that we will be using it that the temperature of the remote upstream reactants is small compared to the activation temperature of the reaction. Since the activation temperature is also the temperature scale, this then requires that the remote upstream temperature is zero to leading order. Since the remote burned state must be a singular point of the system the reaction rate there must be zero. This can be accomplished by taking gases far downstream as fully burned. In order that the "regular" solution is found, we will specify that far upstream of the flame the balance in the energy equation is between conduction and convection with reaction being much smaller. This will prevent any "fast" deflagration wave solutions (see Kassoy, 1985, for example, for a discussion of fast deflagration waves, that is deflagration waves where the remote upstream balance in the cold reactant gas stream is between convection and reaction) from appearing. As a result, some of the

boundary conditions are

$$T(-\infty) = 0,\ Y(-\infty) = Y_{\infty},\ Y(+\infty) = 0,\ dT/dx \to 0 \quad \text{as} \quad x \to +\infty,$$
$$(d^2T/dx^2)/(M\,dT/dx) \to 1 \quad \text{as} \quad x \to -\infty. \tag{15}$$

Before we discuss the rest of the boundary conditions necessary to produce a unique solution, we will investigate how the boundary conditions used so far influence the choice of integration constant in (12). As $x \to -\infty$, the mass flux M must approach $(d^2T/dx^2)/(dT/dx)$ and so for large negative x

$$P(T(T''/T')')'' - (T(T''/T')')'(T''/T') + T((T''/T')')^2 \simeq K. \tag{16}$$

where $'$ denotes derivatives with respect to x and K is the constant of integration in (12). If any of the three terms approaches a non-zero constant as $x \to -\infty$, then all the terms become of the same order of magnitude and T grows quartically. In fact, an exact solution to (16) is given by $T = Kx^4/(27 - 6P)$. From this we can get the rest of the unknowns (u, v, p, ϱ) for an exact solution to a viscous, conducting incompressible flow problem.

The only other way to have the left hand side approach a constant is if two of the terms become very large but their sum approaches a constant. This becomes impossible because if two of the terms become of the same order of magnitude, then it is easily determined that T must attain quartic growth as before. This then implies that the only permissible value of the constant is zero and so now our set of three governing equations is (12–14) with the constant for equation (12) being 0. This condition implies that there is no transverse pressure gradient.

The physical reason why there cannot be a non-zero transverse pressure gradient is that the density ratio of the hot product gas stream to the cold reactant stream becomes infinite in the large heat release limit. Therefore the interface between the hot and cold gases behaves in a manner similar to the liquid–gas interface of a rising bubble (*i.e.*, free streamline theory). A practical combustion problem that may have this character is a premixed flame attached to a bluff body. In that configuration the flame sheet roughly separates cold, high momentum fluid in the free stream from hot, low momentum fluid in the recirculation zone. Since the density difference between the freestream and the wake can be large, say a factor of 7 or 8, the separation streamline might be profitably considered as a free streamline. Since the wake gasses are so slowly moving in the recirculation zone of an attached premixed flame, it may be better to analyze the flame structure through the limit given here rather than through a boundary layer analysis where the speed of the remote reactants is taken to be very much larger than the local flame speed.

THE REMOTE BURNED STATE

An analysis of appropriate to the remote burned state can also be performed. In this case we will transform the problem into a phase space with T as the independent variable through the definition

$$z \equiv dT/dx \tag{17}$$

to arrive at the set of equations

$$Pz\, d(z\, d(Tz\, dM/dT)/dT)/dT - Mz\, d(Tz\, dM/dT)/dT + Tz^2(dM/dT)^2 = 0 \quad (18)$$

$$M = dz/dT + Q\, T^{m-1}\, Y \exp(-1/T)/z \quad (19)$$

$$M\, dY/dT = (1/L)\, d(z\, dY/dT)/dT - T^{m-1}\, Y \exp(-1/T)/z \quad (20)$$

and the partial set of boundary conditions (15) become

$$Y(0) = Y_0, \quad Y(T_f) = 0, \quad z(0) = 0, \quad z(T_f) = 0,$$

$$(dz/dT)/M \to 1 \quad \text{as} \quad T \to 0 \quad (21)$$

where T_f is the final temperature of the burned gases. T_f is to be determined as part of the solution.

We will now look for solutions to this system in the neighborhood of the point $T = T_f$, $Y = 0$, $z = 0$, $M = M_0$ through the leading order expansions

$$T = T_f + \varepsilon\tau, \quad z = \varepsilon\zeta, \quad Y = \varepsilon y, \quad M = M_0 + \delta m, \quad \varepsilon \ll 1, \quad \delta \ll 1 \quad (22)$$

appropriate to this problem.

The system governing the behavior in the far field is

$$d\zeta/d\tau = M_0 - Q\, T_f^{m-1}\, y \exp(-1/T_f)/\zeta \quad (23)$$

$$d(\zeta\, dy/d\tau)/d\tau = L(M_0\, dy/d\tau + T_f^{m-1}\, y \exp(-1/T_f)/\zeta) \quad (24)$$

$$d^3m/d\tau^3 = -3(d\zeta/d\tau)(d^2m/d\tau^2)/\zeta - (d\zeta/d\tau)^2\,(dm/d\tau)/\zeta^2 - (d^2\zeta/d\tau^2)(dm/d\tau)/\zeta$$

$$+ M_0((d\zeta/d\tau)(dm/d\tau)/\zeta^2 + (d^2m/d\tau^2)/\zeta)/P \quad (25)$$

with initial conditions

$$\zeta(0) = y(0) = m(0) = 0. \quad (26)$$

The general solution to this underdetermined non-linear system is

$$\zeta = A\tau \quad (27)$$

$$y = B\tau \quad (28)$$

$$m = C|\tau|^{\alpha} \quad (29)$$

where

$$A = (LM_0 - \sqrt{(L^2M_0^2 + 4LQ)})/2 \quad (30)$$

$$B = M_0(1 - L)/A\, Q\gamma - L/Q \quad (31)$$

$$\alpha = M_0 AP \tag{32}$$

$$\gamma = T_f^{-1} \exp(-1/T_f) \tag{33}$$

and C is arbitrary. Casting the solution back into the original variables we then get the approximate solution

$$z \approx A(T - T_f) \tag{34}$$

$$Y \approx B(T - T_f) \tag{35}$$

$$M \approx M_0 + C(T_f - T)^2 \tag{36}$$

if we take

$$\delta = \varepsilon^2. \tag{37}$$

A number of points can be addressed with this solution for the far field structure. If the solution for the perturbation to the mass flux, m, is to make any sense we must have $\alpha > 0$ or $C = 0$. In the case where $C = 0$ we can take δ as an arbitrarily small scale compared to ε. This then implies that the variation in M within the ε neighborhood of $T = T_f$ is identically zero and so every derivative of M with respect to T must vanish at $T = T_f$. We therefore know that M must be identically zero in some finite neighborhood of $T = T_f$ or else it has an essentially singularity at $T = T_f$. Numerical calculations on the full Eqs. (18–20) indicate the former and furthermore show that M is identically constant from $T = 0$ to $T = T_f$. Of course the boundary conditions at $T = 0$ are not met in general, but for a specific choice of M_0 they are. That choice is the adiabatic burning rate.

Since our interest is in the effects of flow non-uniformities, and therefore varying M, attention must be placed on the case where $C \neq 0$. When this happens we must conclude that M_0 is negative in order that α is positive. The reason for this is that as $x \to \infty$ either T' is positive and T'' is negative of T' is negative and T'' is positive if T approaches a constant value. This implies that dz/dT (which is the same as T''/T') must be negative at $T = T_f$. We therefore know that A is negative. Of course, the Prandtl number P is positive and hence if α is to be positive then M_0 must be negative. This result is not too surprising. A more interesting conclusion can be reached once the condition of non-negative mass fractions is applied. In the far field the imposition of non-negative mass fraction requires that $B \leqslant 0$. This will be true for any negative value of M_0 if $L \geqslant 1$ but will not be true in general if $L < 1$. When $L < 1$ a critical mass flux $+\infty$ given by

$$M_{0C} = -\sqrt{L\gamma}/(1 - L) \tag{38}$$

can be uncovered. B vanishes at this particular value of M_0. If M_0 is smaller than M_{0C}, then B as defined by (31) becomes positive and hence the mass fraction of reactant becomes negative in the far field. Since this is impossible, we must have

$$-\sqrt{L\gamma}/(1 - L) \leqslant M_0 \leqslant 0 \tag{39}$$

when $L < 1$.

The inequality (39) can be rewritten in the form

$$T_f^{n-1} \exp(-1/T_f) \geq (1 - L) M_0^2 L \geq 0. \tag{40}$$

If $n > 1$, then the left hand side of (40) is a monotonically increasing function of T_f that increases without bound. For a given value of M_0 and Lewis number less than one, a minimum possible burned gas temperature is predicted. This situation is of limited interest because it corresponds to a reaction rate that increases without bound with temperature. This is hardly realistic in that for sufficiently high temperatures the fraction of collisions that have the requisite amount of energy approaches one while the density of the reactants approaches zero. We therefore know that the rate of reaction must go to zero as the temperature goes to infinity.

In the case where $n = 1$, again a minimum burned gas temperature is predicted but the left hand side of (40) no longer grows without bound. Since the left hand side of (40) is bounded between 0 and 1 for all positive values of T_f, M_0^2 is bounded between 0 and $L/(1 - L)$. In this case a minimum value of M_0 is predicted, namely $-\sqrt{L/(1 - L)}$, that is attained at an infinite flame temperature. At any finite flame temperature the value of M_0 must be higher. Again this case is of limited interest because now the rate of reaction goes to a positive constant instead of zero as the temperature goes to infinity.

When $n < 1$ the left hand side of (40) is no longer monotone but achieves a maximum value at a finite temperature. This again puts a bound on M_0 but now the minimum value is achieved at a finite temperature.

This predicts a maximum possible amount of blowing from behind, that is a minimum possible value of M_0, if the Lewis number is less than one and the reaction constant n is less than or equal to one so that the rate of reaction approaches zero as the temperature becomes infinite. This lower bound on M_0 is surprisingly independent of the composition of the fresh mixture. The maximum possible value of $|M_0|$ is attained at a final burned gas temperature of $1/(1 - n)$ and has a value of

$$|M_0|_{max} = \sqrt{L}(1 - n)^{n-1} \exp(n - 1)/(1 - L) \tag{41}$$

This means that as the blowing from behind the flame is increased, extinction must occur at or before the value of the blowing given by (41) if both L and n are less than one.

The physical reason for the restriction on n is that when n is less than one, the reaction rate eventually begins to fall as the temperature rises. For large enough temperatures the drop in overall concentration with rising temperature overwhelms the increase in the concentration of sufficiently energetic molecules as represented by the exponential term. This behavior can appear for Lewis numbers less than one because the blowing from behind increases the temperature of the mixture, a fact that has been confirmed through numerical integration of the governing equations. Sufficiently large amounts of blowing can conceivably raise the temperature to the point where the reaction rate begins to fall due to a sufficiently large drop in density. This effect is the reason for the restriction (41). This type of extinction mechanism cannot be studied through the use of AEA since it can only occur when the final gas temperatures are of the same order of magnitude as the activation temperature.

Here we have taken the mass flux of the remote opposed flow to be finite and yet in the AEA/boundary layer solutions the magnitude of the mass flux appears to grow without bound. There is no inconsistency, however. In the AEA solutions the velocity scale is the adiabatic flame speed whereas here we have used a velocity scale that

normalizes the coefficient of the reaction term. The AEA solutions, where the temperature of the remote reactants is small, can be recovered by restricting T_f to be small and taking M_n to be large compared to the adiabatic burning rate. This is possible even though the critical value of M_n approaches zero as T_f goes to zero because the critical mass flux is $O(\sqrt{\gamma(T_f)})$ whereas the adiabatic burning rate is $O(\sqrt{\gamma(T_f)}/T_f)$ and so the critical mass flux is much larger.

Arrhenius kinetics are not an essential feature fo this extinction mechanism. If we use a reaction rate temperature dependence of the form $f(T)$ where $f(0) = 0$, $f(T) \to 0$ as $T \to \infty$, $f(T) > 0$ for $T > 0$, and $f(T)$ continuous then we can derive the result that

$$M_n^2 \leqslant Lf(T_f)/(1 - L) \tag{42}$$

when the Lewis number L is less than one. These restrictions on $f(T)$ are all physically realistic in that we expect essentially zero rate of reaction for small temperatures, diminishing rate of reaction for very high temperatures since the fraction of sufficiently energetic molecules can become no higher than one and the concentration of reactants must decrease with temperature, and the rate of reaction must always be positive. Since the physically realistic restrictions imposed on $f(T)$ imply that $f(T)$ has a maximum value, we can therefore conclude that there is a maximum amount of blowing that a flame with Lewis number less than one can withstand and this maximum is no greater than that predicted by (42).

Although an extinction mechanism like this is predicted mathematically, the question remains as to whether or not it is physically accessible. In addition, it is possible that the failure of a physically realistic flat-flame similarity solution to exist only indicates that the solution bifurcates or jumps to a nonplanar solution. A complete answer to these questions would require the study of a complete reaction mechanism, large scale numerical simulations, developing appropriate existence and uniqueness theorems, experimental investigation, or some combination. Such a task is beyond the scope of this work.

CONCLUDING REMARKS

Here we have shown that there exists a potential mechanism for the abrupt extinction of aerodynamically strained premixed flames with Lewis numbers less than one. The surprising feature of this mechanism is that instead of the usual notion of a flame extinguishing by becoming too cold, here flames can extinguish by becoming too hot.

The physics of this mechanism is surprisingly simple. When the Lewis number of a combustible mixture is less than one, aerodynamic straining of the flame will cause a rise in flame temperature. Eventually the rate of reaction must fall due to the fact that the concentration of active species is inversely proportional to the temperature (if the pressure is fixed) and the fraction of sufficiently energetic collisions can be no greater than one. This falling reaction rate with increased blowing can extinguish the flame.

The question remains as to whether or not this extinction mechanism is accessible to physical flames. Perhaps a simple experiment can reveal the answer.

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APPENDIX B

Xerox copy of a manuscript that appeared in the Springer-Verlag Lecture Notes in Physics Series, v 299, entitled

"High Temperature Extinction of Premixed Flames"

by

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HIGH TEMPERATURE EXTINCTION OF PREMIXED FLAMES

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ABSTRACT

The far field of a stretched premixed flame with A→B⇌C kinetics is studied. Each of the reaction rates are assumed to be proportional to the mass fraction of the reactants and have a temperature dependence that is continuous, positive, and vanishes at both infinite and zero absolute temperature. Arrhenius reaction rate functions are examples that satisfy these requirements. Bounds are uncovered for the amount of blowing from behind the flame that plane premixed flames can withstand for all Lewis numbers when the intermediate species are lighter than the deficient reactant. When the intermediate products are heavier than the deficient reactant, bounds on the blowing are found when the Lewis number of the deficient reactant is less than one.

INTRODUCTION

Through the analysis of the far field of adiabatic stretched premixed flames with A→B kinetics, we have been able to show that premixed flames with Lewis numbers less than one will be extinguished given sufficiently strong blowing from behind [1]. This is inferred from the analysis in that the mass fraction of combustible becomes negative in the far field if the opposed flow is above a maximum allowable level. The activation energy asymptotic (AEA) analyses of this case [2-7] do not show true extinction. What we mean by true extinction is the failure of existence for a flame structure for sufficiently strong opposed flow.

In the previous work [1] it was unclear as to what effect dissociation would have on the results. Here we will investigate a kinetic mechanism that incorporates dissociation. The simplest possible reaction mechanism that would include dissociation is A⇌B.

It seems unlikely that the analysis of such a mechanism would reveal anything of interest in that the final equilibrium state would be composed of major species only without any intermediates. A more plausible model is the A-B-C mechanism where B represents intermediate products and the final equilibrium state is dominated by intermediate and final products.

The plan of this paper is to first analyze the far field of the stretched A-B-C flame so that the case without dissociation is fully documented. Once the non-dissociating model is fully explored we shall include the effects of dissociation.

MATHEMATICAL MODEL

The equations that model two-dimensional, low Mach number combustion waves under the assumption of calorifically and thermally perfect gases with constant transport properties are

$$\partial(\rho u)/\partial x+\partial(\rho v)/\partial y=0 \tag{1}$$

$$\partial(\rho uT)/\partial x+\partial(\rho vT)/\partial y=\nabla^2 T+q_1 Yf_1(T)+q_2 Xf_2(T)-q_2 Zf_3(T) \tag{2}$$

$$\partial(\rho uY)/\partial x+\partial(\rho vY)/\partial y=(L_A)^{-1}\nabla^2 Y-Yf_1(T) \tag{3}$$

$$\partial(\rho uX)/\partial x+\partial(\rho vX)/\partial y=(L_B)^{-1}\nabla^2 X+Yf_1(T)-Xf_2(T)+Zf_3(T) \tag{4}$$

$$Z=1-X-Y \tag{5}$$

$$\rho u\partial u/\partial x+\rho v\partial u/\partial y=-\partial p/\partial x+P(\nabla^2 u+(\partial(\partial u/\partial x+\partial v/\partial y)/\partial x)/3) \tag{6}$$

$$\rho u\partial v/\partial x+\rho v\partial v/\partial y=-\partial p/\partial y+P(\nabla^2 v+(\partial(\partial u/\partial x+\partial v/\partial y)/\partial y)/3) \tag{7}$$

$$\rho=1/T. \tag{8}$$

u and v are the non-dimensionalized x and y components of fluid velocity, T is the non-dimensional temperature, ρ is the non-dimesional density, p is the non-dimensional pressure, P is the Prandtl number and X, Y and Z are the mass fractions of the intermediate product, the reactant and the final product respectively. These equations are continuity (1), energy balance (2), species balance (3-5), x and y momentum balance (6-7) and equation of state (8).

Proceeding as in [1], this system can be simplified for plane flames in a non-uniform flow field. The resulting equations under the limit of large heat release are

$$MdT/dx=d^2T/dx^2+q_1 Yf_1(T)+q_2 Xf_2(T)-q_2(1-X-Y)f_3(T) \tag{9}$$

$$MdY/dx=(1/L_A)d^2Y/dx^2-Yf_1(T) \tag{10}$$

$$MdX/dx=(1/L_B)d^2X/dx^2+Yf_1(T)-Xf_2(T)+(1-X-Y)f_3(T) \tag{11}$$

$$Pd^2(TdM/dx)/dx^2-Md(TdM/dx)/dx+T(dM/dx)^2=0. \tag{12}$$

M is the mass flux, ρu. Without the limit of large heat release

$(T_{flame}/T_{remote\ reactants} >> 1)$ the right hand side of equation (12) could be a non-zero constant.

Appropriate boundary conditions are

$$T(-\infty)=X(-\infty)=0,\ Y(-\infty)=Y_{-\infty},\ T(+\infty)=T_f,\ M(+\infty)=M_o$$
$$X(+\infty)=f_3(T_f)/(f_2(T_f)+f_3(T_f)),\ Y(+\infty)=0 \tag{13}$$

where T_f is the temperature of the remote products, a quantity that must be found as part of the analysis. In addition, a boundary condition is needed to force the balance in the remote reactants to be one between conduction and convection without appreciable reaction. Such a condition is

$$(d^2T/dx^2)/(M\ dT/dx) \to 1 \text{ as } x \to -\infty. \tag{14}$$

THE REMOTE BURNED STATE

Since the system (9-13) is autonomous, we can transform the problem into a phase space problem on a finite domain with independent variable T through the definition

$$z = dT/dx. \tag{15}$$

The resulting system of equations is

$$M = dz/dT + (q_1Yf_1(T) + q_2Xf_2(T) - q_2(1-X-Y)f_3(T))/z \tag{16}$$
$$MdY/dT = (1/L_A)\ d(zdY/dT)/dT - Yf_1(T)/z \tag{17}$$
$$MdX/dT = (1/L_B)\ d(zdX/dT)/dT + (Yf_1(T) - Xf_2(T) + (1-X-Y)f_3(T))/z \tag{18}$$
$$Pzd(zd(TzdM/dT)/dT)/dT - Mzd(TzdM/dT)/dT + Tz^2(dM/dT)^2 = 0 \tag{19}$$

and the boundary conditions at $x=+\infty$ become

$$z(T_f)=0,\ X(T_f)=f_3(T_f)/(f_2(T_f)+f_3(T_f))=X_f,$$
$$Y(T_f)=0,\ M(T_f)=M_o. \tag{20}$$

Near $T=T_f$ we can write

$$z = \epsilon\zeta,\ Y = \epsilon\psi,\ X = X_f + \epsilon\xi$$
$$T = T_f + \epsilon\tau,\ M = M_o + \delta\mu. \tag{21}$$

The resulting system is

$$M_o = d\zeta/d\tau + q_1\psi f_1(T_f) + q_2[\tau\Lambda(T_f) + \psi f_3(T_f) + \xi(f_2(T_f)+f_3(T_f))] \tag{22}$$
$$M_o\ \zeta\ d\psi/d\tau = (1/L_A)\ \zeta\ d(\zeta\ d\psi/d\tau)/d\tau - \psi f_1(T_f) \tag{23}$$
$$M_o\ \zeta\ d\xi/d\tau = (1/L_B)\ \zeta\ d(\zeta\ d\xi/d\tau)/d\tau + \psi f_1(T_f) - \xi(f_2(T_f)+f_3(T_f)) - \psi f3(T_f) - \tau\Lambda(T_f) \tag{24}$$

and another equation for μ that is of no consequence in the remainder of the analysis. The function Λ is defined by

$$\Lambda(T) = (f_3\ df_2/dT - f_2\ df_3/dT)/(f_2 + f_3). \tag{25}$$

The boundary conditions are

$$\zeta(0)=\psi(0)=\xi(0)=0. \tag{26}$$

The singular point described by the system (22-24, 26) is inherently non-linear, but fortunately it admits solutions of the form

$$\psi = ar,\ \xi = br,\ \zeta = cr. \tag{27}$$

Substitution into (22-24) results in

$$c = [L_A M_o - \sqrt{(L_A M_o)^2 + 4L_A f_1(T_f)}]/2 \tag{28}$$

and the set of algebraic equations

$$a(q_1 f_1(T_f)+q_2 f_3(T_f)) + bq_2(f_2(T_f)+f_3(T_f)) = M_o c - c^2 - q_2\Lambda(T_f) \tag{29}$$

$$a(f_1(T_f)-f_3(T_f)) + b(c^2/L_B - M_o c - f_2(T_f) - f_3(T_f)) = \Lambda(T_f) \tag{30}$$

that are trivially solved for a and b so that a,b and c are now known as functions of M_o and T_f. There is another solution for c with the positive root in (28), but that solution is not consistent with the fact that T approaches a constant as x goes to infinity.

THE REMOTE SINGULAR POINT FOR NO DISSOCIATION

The solution fails to be physically realistic when a is positive since that would correspond to a negative mass fraction for Y near the singular point. The case where a=0 therefore defines a critical condition.

The specification of the critical condition is very simple in the case of no dissociation. When dissociation is neglected we must take $f_3(T)=0$ which implies that $\Lambda=0$. Setting a equal to zero and eliminating b from (29-30) gives rise to

$$(M_o c(1-L_A)-f_1(T_f)L_A)(M_o c(L_A/L_B - 1)+L_A/L_B\ f_1(T_f)-f_2(T_f))=0. \tag{31}$$

Substituting (28) for c gives the two critical conditions

$$M_o{}^2{}_c = L_A f_1(T_f)/(1-L_a) \tag{32}$$

and

$$M_o{}^2{}_c = (f_2(T_f)-L_A/L_B\ f_1(T_f))^2/[L_A(f_2(T_f)-f_1(T_f))(L_A/LB-1)]. \tag{33}$$

Since the Lewis numbers and reaction rates are always positive, condition (32) can only be attained when $L_A < 1$. In addition, if we only consider the case where $f_2(T) > f_1(T)$ throughout the range of possible final product temperatures T_f so that product formation is a faster reaction than the breakdown of the reactants (usually a good assumption since the breakdown of the relatively stable reactants is governed by a fairly high activation temperature mechanism and the formation of product from intermediates is typically through reactions with small activation temperatures), then condition (33) can only apply if $L_A > L_B$. This is a very common occurence since it requires, roughly speaking, the mean molecular weight of the intermediate species to be smaller than the molecular weight of the deficient

reactant. The only potential mechanism that we can think of that does not conform to this condition is lean hydrogen oxidation where the deficient reactant has molecular weight 2 and the intermediate species are H, OH and O. It is likely that the mean molecular weight of the intermediates will be greater than 2 in this case.

Condition (32) is identical to the critical condition for the A→B mechanism [1].

An example where $L_B < L_A$ and $L_A > 1$ is given in Figure 1. This situation occurs when the intermediate products are ligther than the deficient reactant and the deficient reactant is heavier than the bulk gas. In this case only (33) defines a limiting condition. In this and all subsequent figures, the shaded regions are regions in the parameter plane where the remote reactant mass flux is mathematically negative and hence is of no physical significance.

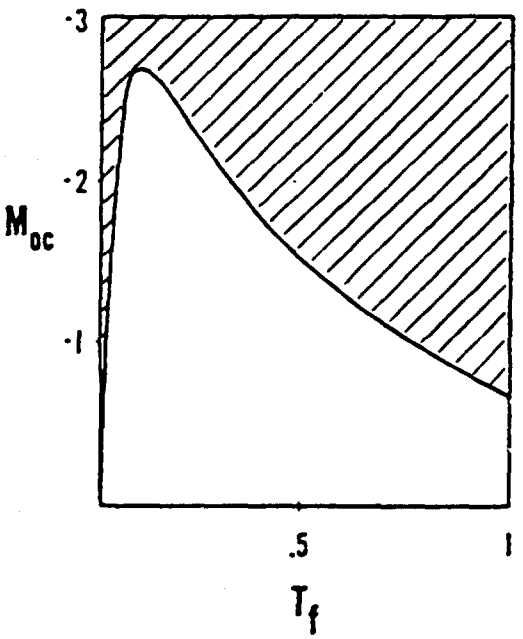

Fig. 1: Critical remote mass flux versus flame temperature. L_A=1.2, L_B=.8, q_1=-1, q_2=2, f_1=exp(-1/T)/T, f_2=exp(-.1/T)/T

Figure 2 shows a case when $L_A < 1$ and $L_A < L_B$. Since this case only applies to the situation where the deficient reactant is both lighter than the intermediate products and the bulk gas, it seems likely that it may only apply to lean hydrogen/oxygen or lean hydrogen/oxygen/diluent mixtures. In this case only the condition (32) applies.

Figure 3 shows a case where $L_B < L_A < 1$. Such a situation is likely for lean methane/air flames, for example, where the prin-

ciple intermediates are lighter than the deficient reactant which in turn is lighter than the bulk fluid. In this case critical conditions are given by both (32) and (33).

In the first two cases it is clear that there are no physically realizable solutions if the remote mass flux in the burned gas becomes too high. In the last case shown in Figure 3, the mass fraction of the remote reactants is positive if conditions are such that the

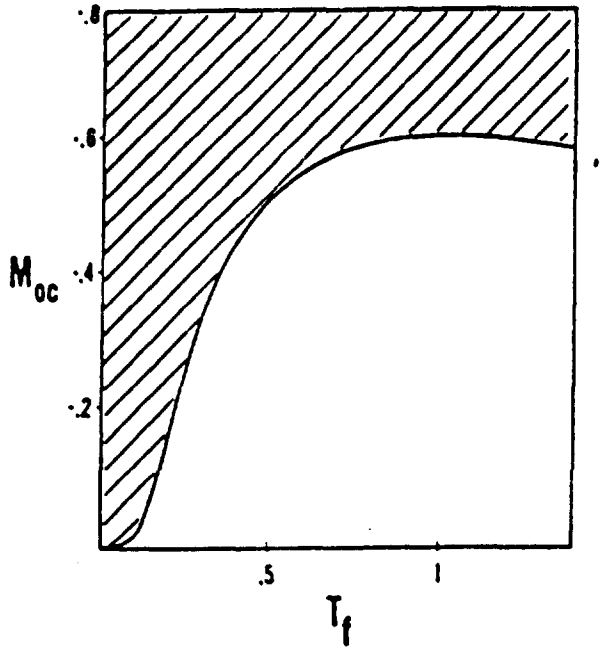

Fig. 2: Critical remote mass flux versus flame temperature. L_A=.5, L_B=.7, q_1=-1, q_2=2, f_1=exp(-1/T)/T, f_2=exp(-.1/T)/T

flame is above both curves. As a practical matter, however, such solutions are probably not accessible since the starting conditions in any real system would be in the lower domain and there is no way to enter the upper domain in any continuous manner except through the single point where the two domains meet. The "solution" at the point where the two solutions meet is found as limit of problems where the remote upstream reactant mass fraction goes to zero and hence is not truly a flame. In fact, the solid curves are not part of the region of physically realistic flame solutions because they correspond to situations where the remote upstream mass fraction of reactant is zero and hence there is no flame. This fact is found through numerical integration of the governing equations.

THE REMOTE SINGULAR POINT WITH DISSOCIATION

When dissociation is retained, the critical M_o is found by solving the algebraic equation

$$(CM_o(1-L_A)-L_A f_1(T_f)-q_2\Lambda(T_f))(CM_o(-1+L_A/L_B)+f_1(T_f)L^A/L_B -f_2(T_f)-f_3(T_f)) = q_2\Lambda(T_f)(f_2(T_f)+f_3(T_f)) \quad (34)$$

where C, a function of M_o, is given by (28). This is done most easily by numerical root finding.

First we will consider the case where $L_B < L_A$ and $L_A > 1$, such as a lean heavy hydrocarbon/air premixed flame, with weak dissociation.

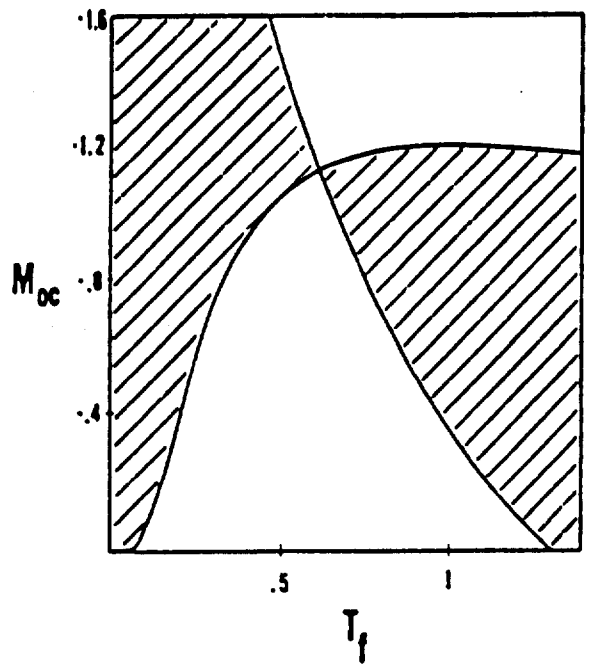

Figure 3: Critical remote mass flux versus flame temperature. L_A=.8, L_B=.4, q_1=-1, q_2=2, f_1=exp(-1/T)/T, f_2=exp(-.1/T)/T

A typical parameter plot is shown in Figure 4. Comparing this plot to the corresponding case without dissociation (Figure 1) we see that dissociation decreases the maximum amount of blowing that the flame can withstand.

In the case where $L_A < L_B < 1$, as shown in Figure 5, the maximum possible amount of blowing is increased through the action of dissociation. As mentioned earlier, such an ordering of the Lewis numbers is very infrequent in applications. One of the only possible physical systems that might have such an ordering is lean hydrogen/air premixed flames.

The case where $L_B < L_A < 1$ is shown in Figure 6. This manner of

Lewis number ordering is characteristic of rich propane or heavier hydrocarbon/air mixtures. It is interesting to note that there is no longer a maximum amount of blowing predicted by the analysis of the

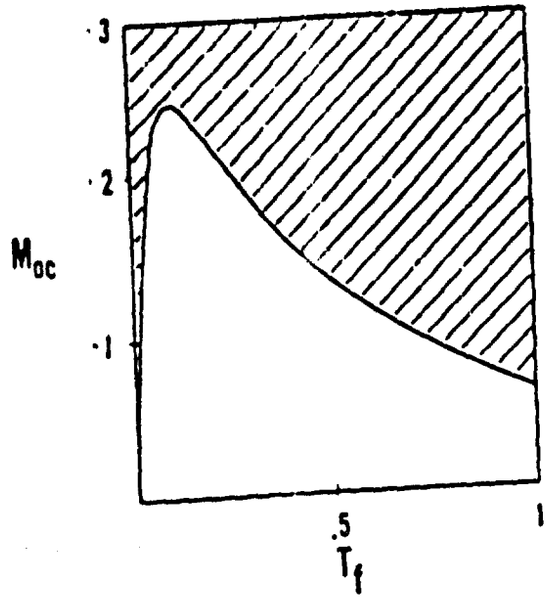

Figure 4: Critical mass flux versus flame temperature
L_A=1.2, L_B=.8, q_1=-1, q_2=2, f1=exp(-1/T)/T
f_2=exp(-.1/T)/T, f_3=.001 exp(-2/T)/T

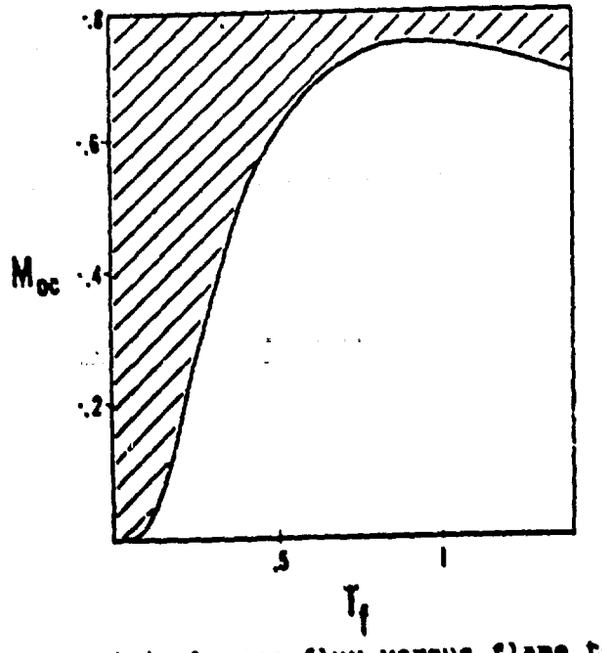

Figure 5: Critical mass flux versus flame temperature.
L_A=.5, L_B=.7, q_1=-1, q_2=2, f_1=exp(-1/T)/T
f_2=exp(-.1/T)/T, f_3=exp(-2/T)/T

remote burned state. A gap opens up through which solution curves may pass and the stronger the rate of dissociation, the wider the gap. It is probable, though we hasten to add that we have not checked this result fully, that the situation can arise where near stoichiometric mixtures will extinguish with sufficiently high blowing but rich mixtures will not with some pivotal value of the remote mass fraction of reactant, denoted by Y_c, that seperates the two cases. This phenomena is shown schematically in Figure 7. As the rate of dissociation is increased, the gap should widen with a subsequent increase in the pivotal value of the remote reactant mass flux. With a sufficiently high rate of dissociation, it seems likely that the pivotal value of the mass fraction of reactants should go to 1 with further increases in the rate of dissociation resulting in no maximum rate of blowing.

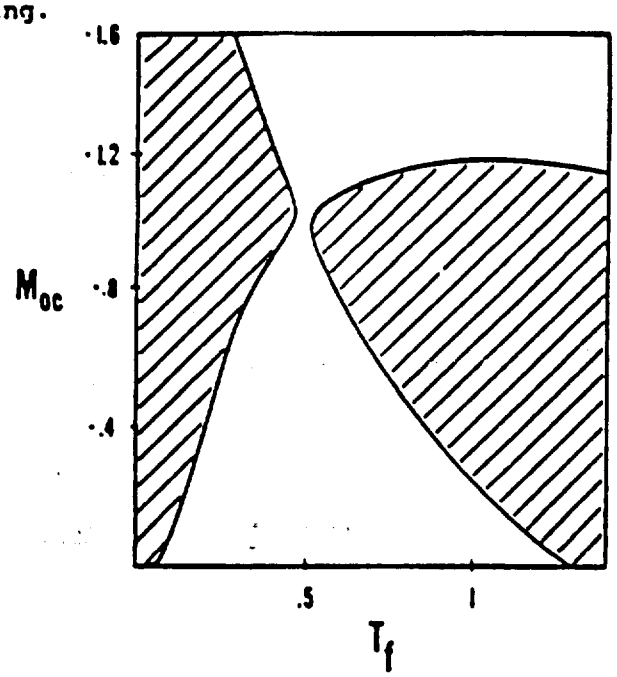

Figure 6: Critical mass flux versus flame temperature.
L_A=.8, L_B=.4, q_1=-1, q_2=2, f_1=exp(-1/T)/T
f_2=exp(-.1/T)/T, f_3=.001 exp(-2/T)/T

CONCLUDING REMARKS

Here we have analyzed the response of a plane premixed flame with sequential kinetics to a non-uniform flow field. Two seperate cases were investigated; one where the second step was irreversible and one where it was reversible. The inclusion of reversibilty in the second step did not alter the qualitative flame response except in the case

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