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THE SINGULAR PERTURBATION APPROACH TO FLAME THEORY
WITH CHAIN AND COMPETING REACTIONS

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ABSTRACT

We investigate the structure of laminar flames with two chemical reactions in the limit of high activation energy asymptotics. Depending on the specific reaction network and the other given chemical data, a wide variety of flame configurations are possible. Here we fully explore these possibilities in the case of sequential and competing reaction pairs. Our methods are general enough to extend to most reaction networks with two or three exothermic reactions with high activation energy.

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DISCLAIMER

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Combustion theory provides an extremely fertile ground for asymptotic analysis. This is due in part to the fact that the theory combines fluid dynamics and chemical reaction theory, both in themselves rich in difficult problems, and in part to the prevalence of small and large parameters appearing in the underlying equations.

One of the most notable large parameters expresses the fact that in combustion problems, the rates of some important chemical reactions typically depend very strongly on the temperature. In the context of the simplest cases of steady plane laminar flame theory, this fact results in a problem of the form [2]

$$L U = f\left(\frac{U-U_+}{\varepsilon}, \varepsilon\right)$$

where ε is a small parameter. Here L is a (vector valued) second order differential operator in the space variable x which does not depend on ε , and U_+ is some reference vector. The solution of this problem has the following "layer" feature: the derivative U' undergoes an abrupt change with magnitude order of unity (as $\varepsilon \rightarrow 0$) in a small interval with length order of ε . This interval is called a flame layer because it is here, and only here, that the source (reaction) term f has a significant effect. The function U , therefore, can be approximated for small ε by a function with derivative discontinuous at one point.

This latter piecewise smooth function itself satisfies a boundary value problem (the "reduced problem") in which the parameter ε no longer appears: the nonlinearity has been replaced by a condition specifying the jump in U' at its point of discontinuity (i.e., across the flame).

The above description holds when there is only one chemical reaction in the flame process, and it is exothermic with high activation energy. See [1],[3] for a comprehensive treatment. When there is more than one reaction, the situation outlined above must be modified. Depending on the specific reaction network and the other given chemical data, a wide variety of flame configurations become possible. In this paper we shall explore these possibilities in the case of sequential and competing reaction pairs. In the former case there is some overlap of our results with those of

Kapila and Ludford [4]. Pairs of reactions have also been considered in [5-8]. Cases were treated in [6-8] which are in some sense limiting cases of those described here. A much fuller account of our results will be given in [9]. In particular, the latter paper contains an extension of our methods to flames with competing-fuel reaction pairs. They admit immediate extension to most reaction networks with two or three exothermic reactions with high activation energy.

Our analysis is largely formal, although great care is taken to justify the approximations made. They are based on the smallness of certain parameters ε_i . Often, other parameters will be assumed to be "order of unity" or "O(1)". This concept means these parameters are neither very large nor very small; otherwise, it is left without strict definition. Effectively, it means that the error introduced by an approximation should be estimable in terms of some ε_i , or a positive power of it, multiplied by a coefficient which depends on these other parameters. The other parameters, therefore, should not be so large or small as to vitiate the accuracy of the approximation.

We begin with a description of the asymptotics and reduced problem for the standard case of a single reaction.

1. Simple Flames

Without giving the physical derivation, we simply write the basic problem for laminar flames with a single reaction $A \rightarrow P$. We call them simple flames. Here $U = \begin{bmatrix} T \\ Y \end{bmatrix}$, T and Y are dimensionless temperature and concentration of reactant A , respectively. The problem is to determine the "profile" $U(x)$ and the mass flux M from the conditions

$$DU'' - MU' = -\omega(U)K, \quad (1a)$$

$$U(-\infty) = U_{\infty}, \quad Y(\infty) = 0. \quad (1b)$$

Here D is a positive definite transport matrix which is taken for simplicity to be constant (this is not necessary [3]), K is the vector

$[_{-}^Q]$, and w is a reaction rate, which we take to be of Arrhenius type:

$$w = B Y e^{-E/T} , \quad (2)$$

with B and E (the latter proportional to the "activation energy") positive constants. Throughout this paper, we assume that all elements of matrices such as D , D^{-1} , and vectors K are $O(1)$ (see [3] for more general circumstances).

By integrating (1a) with use of (1b), it is seen immediately that $U(\infty)$ satisfies

$$U(\infty) = U_{+} \equiv \begin{bmatrix} T_{-} + QY_{-} \\ \rho \end{bmatrix} . \quad (3)$$

Thus $T_{+} = T_{-} + QY_{-}$. We assume

$$\varepsilon \equiv T_{+}^2/E \ll 1 \quad (4)$$

and on the basis of this relation, approximate w by

$$w = \frac{\eta}{\varepsilon} \left(\frac{Y}{\varepsilon} \exp [(T - T_{+})/\varepsilon] \right) , \quad (5)$$

where

$$\eta = B \varepsilon^2 \exp (-E/T_{+}) . \quad (6)$$

This approximation is obtained by writing the exponent of (2) as a function of $t = (T - T_{+})/\varepsilon$, and taking the first two terms in its Taylor series expansion in t about $t = 0$. The smallness of ε implies (see [3]) that it can be neglected for temperatures outside a neighborhood of the maximum temperature T_{+} .

We now perform a scale transformation $\bar{x} = x\eta^{\frac{1}{2}}$, $\bar{M} = M\eta^{-\frac{1}{2}}$; (1a) becomes (differentiation is now with respect to $\bar{x}$)

$$D\ddot{U} - \bar{M}\dot{U} = -\frac{1}{\eta} \omega(U)K = -\frac{1}{\varepsilon} \omega^*(u)K \quad (7)$$

where $u = [\frac{t}{y}] = (U-U_+)/\varepsilon$, and

$$\omega^*(u) = \frac{\varepsilon}{\eta} \omega(U) = ye^t \quad (8)$$

We postulate a "reduced problem" of the following form, for $U(\bar{x})$ (assumed continuous) and $\bar{M}$:

$$(DE) \quad D\ddot{U} - \bar{M}\dot{U} = 0 \quad , \quad \bar{x} \neq 0 \quad , \quad (9a)$$

$$(BC) \quad U(\pm\infty) = U_{\pm} \quad (9b)$$

$$(CC) \quad [D\dot{U}]_{0-}^{0+} = -\beta K \quad (9c)$$

Here the scalar β in the "connection condition" (9c) is to be determined a priori by a layer analysis from the function ω^* .

By stretching variables $\xi = x/\varepsilon$, $u = \frac{U-U_+}{\varepsilon}$, and then neglecting the term formally of order ε , we write (7) as

$$Du'' + \omega^*(u)K = 0 \quad (10)$$

This is to be solved for $u = u(\xi)$ under the boundary condition

$$u(\infty) = 0 \quad (11)$$

Since, from (10), u'' is a multiple of $D^{-1}K$ for each ξ , it follows from (11) that u itself must be also:

$$u(\xi) = \sigma(\xi) D^{-1}K \quad (12)$$

Using (12) in (10) and applying (11), we find a problem for σ alone:

$$\sigma'' + \omega^*(\sigma D^{-1}K) = 0, \quad \sigma(\infty) = 0. \quad (13)$$

This has a first integral

$$(\sigma')^2 - \Omega(\sigma) = 0,$$

where $\Omega(\sigma) = 2 \int_{\sigma}^0 \omega^*(sD^{-1}K)ds$. Assuming now that $D^{-1}K$ has first component positive and the second negative, we see from (8) that $\Omega(-\infty)$ exists, can be calculated, and represents $(\sigma'(-\infty))^2$. The matching condition between the flame layer and the "outer" solution is

$$u'(-\infty) = \dot{U}(0-) \quad (14)$$

From this, (12), and the fact that necessarily $U \equiv U_+$ for $\bar{x} > 0$, we may identify the constant β in (9c) as

$$\beta = \sigma'(-\infty) = \left(2 \int_{-\infty}^0 \omega^*(sD^{-1}K)ds \right)^{1/2}. \quad (15)$$

The specification of β completes the definition of the reduced problem (9). What remains is to solve it. To do so, we note, by integrating (9a), that

$$\begin{aligned} [D\dot{U} - \bar{M}U]_{-\infty}^{0-} &= 0 = D\dot{U}(0-) - \bar{M}U_+ + \bar{M}U_- \\ &= \beta K - \bar{M}Y_-K, \end{aligned}$$

hence

$$\bar{M} = \beta/Y_- \quad (16)$$

With $\bar{M}$ known (9a) may now be solved for $\bar{x} < 0$, with known initial conditions at $\bar{x} = 0$. There is a unique solution, and it approaches the correct limit value U_- as $\bar{x} \rightarrow -\infty$. This completes the solution of the reduced problem.

2. The Effects of Other Reactions on Simple Flames

Consider a simple flame profile, as described in Sec. 1, involving a reaction term $w_1(U)K_1$ as in (2), (5), in which the subscript "1" is appended to the quantities ϵ , K , η , E , B , and Y . Thus Y_1 is the concentration of the species A_1 which is exhausted at the flame. We now perturb the problem by adding another reaction, with a concomitant second term w_2K_2 on the right of (1a). Our main result will be a simple criterion for judging whether the second reaction constitutes a negligible perturbation of the given flame. Rescaling with use of η_1 , we obtain the following analog of (7):

$$D\ddot{U} - \bar{M}\dot{U} = -\frac{1}{\epsilon_1} w_1^*(u) K_1 - \frac{1}{\eta_1} w_2(U)K_2 \quad (17)$$

We assume that

$$\epsilon_2 = T_+^2/E_2 \ll 1$$

is also small, so that the effect of w_2 for $\bar{x} < 0$ is negligible, in comparison with its effect in the flame and for $\bar{x} > 0$.

There are two important cases to be considered:

- (I) No reactant for the second reaction is exhausted in the original flame;
- (II) A reactant for the second reaction is also exhausted.

Case I. This case will apply, for example, to our study of sequential reactions in Sec. 3. In this case, w_2 remains strictly positive behind the

flame, and may be represented by

$$\omega_2 = B_2 Y_2 e^{-E_2/T}$$

We are assuming, for simplicity only, that the second reaction, as well as the first, is first order: $A_2 \rightarrow P$. As long as T deviates by amount $o(\varepsilon_2)$ from T_+ , we have

$$\omega_2 \leq C B_2 e^{-E_2/T_+}$$

for some constant $C = O(1)$, and the last term in (17) is bounded in magnitude by

$$q \equiv C B_2 e^{-E_2/T_+} / B_1 \varepsilon_1^2 e^{-E_1/T_+} \quad (18)$$

Since the first term, due to depletion of A_1 , vanishes behind the flame, the effect of the second reaction can be gauged by examining the solution of the initial value problem

$$\ddot{U} - \bar{M}\dot{U} = f(\bar{x}) \quad , \quad U(0) = U_+ \quad , \quad \dot{U}(0) = 0 \quad ,$$

for vectors f with $|f| \leq \nu$. The representation

$$U(\bar{x}) = \int_0^{\bar{x}} \exp[\bar{M}D^{-1}(\bar{x}-s)] D^{-1} f(s) ds + U_+$$

yields

$$|U(\bar{x}) - U_+| \leq C q e^{\lambda \bar{x}} \quad ,$$

for some constants C and $\lambda = O(1)$, since $\bar{M}$ and D^{-1} are $O(1)$ quantities. If, therefore,

$$q = O(\varepsilon_2) \quad ,$$

it follows that $|U(\bar{x}) - U_+| \ll 1$ for $\bar{x} \geq 0$ restricted to any interval of length $O(1)$.

We now define functions

$$H_i(T) = \bar{\varepsilon}(\ln B_i - E_i/T) \quad , \quad (19)$$

where

$$\bar{\varepsilon} = T_+^2 / \text{Min}(E_1, E_2) \quad . \quad (20)$$

It is easily seen that $H_i'(T)$ is at most $O(1)$ for each i , and $H_k'(T_+) = 1$, where k is such that $E_k = \text{Max}[E_1, E_2]$. Suppose, now, that

$$H_2(T_+) - H_1(T_+) = -v < 0 \quad . \quad (21)$$

then from (18),

$$q = \frac{C}{\varepsilon_1^2} e^{-v/\bar{\varepsilon}} \leq C\bar{\varepsilon}^{-2} e^{-v/\bar{\varepsilon}} = o(\varepsilon_2) \quad ,$$

if (for example) v is an $O(1)$ quantity.

Our conclusion is that (21) is a sufficient condition for w_2 to have a negligible effect on the original simple flame in regions a distance $O(1)$ from the flame (actually, it is clear that much larger regions could be allowed).

Case II. In this case, we assume for simplicity that $Y_2 = Y_1 = Y$. A prime example will be the branching network in Sec. 4. The last reaction

rate in (17) becomes

$$\begin{aligned}
\frac{1}{\eta_1} \omega_2 &= \frac{1}{\eta_1} B_2 Y e^{-E_2/T} \\
&\approx \frac{\varepsilon_1}{\eta_1} B_2 e^{-E_2/T_+} y e^{Yt} \\
&= \frac{1}{\varepsilon_1} r \omega_2^*(u) ,
\end{aligned} \tag{22}$$

where we have set

$$Y = E_2/E_1 , \quad \omega_2^* = y e^{Yt} , \tag{23}$$

and

$$r = B_2 e^{-E_2/T_+} / B_1 e^{-E_1/T_+} . \tag{24}$$

We assume $Y = O(1)$ for this exposition. Since Y is depleted, $U = \text{const} = U_+$ for $\bar{x} > 0$, so the stretched variable $u = (U - U_+)/\varepsilon_1$ satisfies the limit condition $u(\infty) = 0$. The layer problem is found from (17), (22), and assumes the form

$$Du'' + \omega_1^*(u)K_1 + r\omega_2^*(u)K_2 = 0 , \tag{25a}$$

$$u(\infty) = 0 . \tag{25b}$$

Reasoning in the same manner as before, we see any solution must be of the form

$$u(\xi) = -\sigma_1(\xi)D^{-1}K_1 - \sigma_2(\xi)U^{-1}K_2 \tag{26}$$

for some scalars σ_j . Substituting into (25), we obtain the problem

$$\sigma_1'' - \omega_1^*(-\sum \sigma_j D^{-1}K_j) = 0 \quad , \quad (27a)$$

$$\sigma_2'' - r\omega_2^*(-\sum \sigma_j D^{-1}K_j) = 0 \quad , \quad (27b)$$

$$\sigma_1(\infty) = 0 \quad . \quad (27c)$$

The following result will be useful to us later, as well as in the present context.

Lemma. Assume the vectors $D^{-1}K_i$ have positive first and negative second components. Then the problem (27) has, for each $r > 0$, a unique (except for translation of the independent variable ξ) positive solution $\sigma_i(\xi)$. It satisfies $-\infty < \sigma_i'(-\infty) < 0$. The quantities $-a_i = \sigma_i'(-\infty)$ depend continuously on r , and satisfy

$$\lim_{r \downarrow 0} \frac{a_2}{a_1} = 0 \quad ; \quad \lim_{r \uparrow \infty} \frac{a_2}{a_1} = \infty \quad . \quad (28)$$

Proof: The equation (2/a,b) may be written as a first order system

$$\sigma_1' = -p_1 \quad ,$$

$$p_1' = -\omega_1^* \quad ,$$

(29)

$$\sigma_2' = -p_2 \quad ,$$

$$p_2' = -r\omega_2^* \quad .$$

The object is to find a trajectory approaching the critical point 0 as $\xi \rightarrow \infty$ from the positive quadrant $P = \{\sigma_i > 0, p_i > 0\}$. It may be checked

that the stable manifold is one dimensional and one branch of it indeed approaches 0 from P. We follow that branch backward: in terms of $s = -\xi$ with " $\dot{\cdot}$ " = " $\frac{d}{ds}$ ", (29) becomes

$$\begin{aligned}\dot{\sigma}_1 &= p_1 \\ \dot{p}_1 &= \omega_1^* \\ \dot{\sigma}_2 &= p_2 \\ \dot{p}_2 &= r\omega_2^* \quad .\end{aligned}\tag{30}$$

Let the positive constants β be defined by

$$D^{-1}K_i = \begin{bmatrix} \beta_{1i} \\ -\beta_{2i} \end{bmatrix} \quad .$$

$$\text{Then for } w = \begin{bmatrix} \sigma_1 \\ p_1 \\ \sigma_2 \\ p_2 \end{bmatrix} \in P \quad ,$$

$$y = \sum_i \beta_{2i} \sigma_i \geq 0 \quad ,\tag{31}$$

so $\omega_1^* \geq 0$. Therefore the right sides of (30) are positive in P, and it follows that the trajectory entering P stays there. In fact, $w(\xi)$ is

monotone increasing, and from (30), (31), we have, for some constants C_i, c_i

$$\sigma_i \geq c_1(s-1)$$

$$y \leq C_2(\sigma_1 + \sigma_2) \quad ,$$

$$t \leq -c_3(\sigma_1 + \sigma_2) \quad ,$$

$$\omega_1^* \leq C_2(\sigma_1 + \sigma_2)e^{-c_3(\sigma_1 + \sigma_2)}$$

$$\leq C_4 e^{-c_5(\sigma_1 + \sigma_2)}$$

$$\leq C_5 e^{-c_6 s} \quad .$$

Hence from (30) again,

$$p_1 \leq C_6 + \int_0^\infty C_5 e^{-c_6 s} ds \leq C_7 \quad .$$

Similar reasoning shows

$$p_2 \leq C_7 \quad .$$

Therefore $p_i(s)$ approach finite limits $a_i = p_i(\infty)$. This proves the first parts of the lemma. We skip the proof of continuity in r . When $r = 0$, the stable manifold we are following backwards lies entirely on the plane $\sigma_2 = p_2 = 0$, so we clearly have $a_2 = 0$, $a_1 > 0$. This establishes the first limit relation (28). For the second, we transform (30) by setting

$s = \bar{s}r^{-\frac{1}{2}}$, $p_i = \bar{p}_i r^{\frac{1}{2}}$, $\sigma_i = \bar{\sigma}_i$, then

$$\dot{\bar{\sigma}}_1 = \bar{p}_1 \quad ,$$

$$\dot{\bar{p}}_1 = \frac{1}{r} \omega_1^*(\bar{\sigma}_1, \bar{\sigma}_2) \quad ,$$

$$\dot{\bar{\sigma}}_2 = \bar{p}_2 \quad ,$$

$$\dot{\bar{p}}_2 = \omega_2^* \quad .$$

As $r \rightarrow \infty$, $\frac{1}{r} \rightarrow 0$ and we use the argument symmetric to the above: it follows that $\bar{p}_1(\infty) \rightarrow 0$, hence $p_1(\infty) = r^{\frac{1}{2}} \bar{p}_1(\infty) \rightarrow 0$. Thus $a_1 \rightarrow 0$, $a_2 > 0$. This gives us the second of (28), and completes the proof.

From (26), we now have

$$Du'(-\infty) = a_1 K_1 + a_2 K_2 \quad .$$

The matching condition is $\dot{U}(0-) = u'(-\infty)$; therefore

$$a\dot{U}(0-) = a_1(r)K_1 + a_2(r)K_2 \quad . \quad (32)$$

This enables us to formulate a reduced problem for Case (11), analogous to (9):

$$DU'' = \tilde{M}\dot{U} = 0, \quad \dot{x} \neq 0 \quad ; \quad (33a)$$

$$U(+\infty) = U_0 \quad ; \quad (33b)$$

and (32). The solution is obtained as follows: from (33a) we have $D\dot{U}(0-) - \bar{M}(U_+ - U_-) = 0$; then from (32) and this,

$$U_+ - U_- = \frac{a_1(r)}{\bar{M}} K_1 + \frac{a_2(r)}{\bar{M}} K_2 \equiv \alpha_1 K_1 + \alpha_2 K_2$$

There are actually two conceivable formulations of the problem here:

- (a) Given U_+ , determine $\bar{M}$, r , and $U(\bar{x})$;
- (b) Given r , determine $\bar{M}$, U_+ , and $U(\bar{x})$.

Of course, either case ignores the fact that r and T_+ are also related through (24), and so (24) will have to serve as a consistency check.

Both problems are solvable. For example in (a), $\alpha_1 > 0$ will be given, so we first determine r from the condition

$$\frac{a_2(r)}{a_1(r)} = \frac{\alpha_2}{\alpha_1} \quad (34)$$

By the lemma (in particular (28)), there exists a value of r which satisfies this relation. It is not clear at this point whether r is unique. Knowing r , we then determine $\bar{M} = a_1/\alpha_1$, and hence $U(\bar{x})$ from (33a).

We now return to the functions H_1 (.9), and suppose that (21) holds. It follows from (24) that $\bar{E} \ln r = -v$, so that

$$r = e^{-v/\bar{E}} \ll 1$$

Therefore by the lemma again, $a_2(r) \ll 1$. But when $a_2 = 0$, the reduced problem (33), (32) is identical to (9), and it is easy to see that the solution depends continuously on a_2 . Hence it is justified to neglect reaction (ii).

Our conclusion, then, is the same as in Case 1: (21) is the criterion by which the second reaction does not significantly alter the original flame. Having developed a general criterion, we proceed to look at specific networks.

3. Reactions in Series

We now consider a combustion process involving a pair of reactions in series:

both exothermic with high activation energy. The unburned state, in the

form $U_- = \begin{bmatrix} T_- \\ Y_{A-} \\ Y_{B-} \end{bmatrix}$ is prescribed. To conceptualize the possible flame structures, we first follow the approach of Sec. 2: we imagine a simple flame resulting from only one of the reactions, the other being artificially suppressed. We then ask whether the criterion is met, whereby the other reaction, if no longer suppressed, would have a negligible effect. If so, then that simple flame is a realizable structure. After this is done, we investigate possible nonsimple flames.

There are four basic simple flames:

F1, produced by reaction (i) only, converting the given unburned state to a partially burned one:

$$U_- \rightarrow U_1 = \begin{bmatrix} T_1 \\ 0 \\ Y_{A-} + Y_{B-} \end{bmatrix}.$$

From (3) it is seen that $T_1 = Q_1 Y_{A-} + T_-$.

F2, produced by (ii) only:

$$U_- \rightarrow U_2 = \begin{bmatrix} T_2 \\ Y_{A-} \\ 0 \end{bmatrix},$$

with $T_2 = T_- + Q_2 Y_{B-}$.

F12, produced by (ii) acting on the product (final state) of F1:

$$U_1 \rightarrow U_+ \equiv \begin{bmatrix} T_+ \\ 0 \\ 0 \end{bmatrix}.$$

where $T_+ = T_- + Q_1 Y_{A-} + Q_2 (Y_{A-} + Y_{B-})$.

F21, acting on the product of F2; here the reaction is of the type $A \rightarrow P$ with rate identical to that of (i), but with heat release equal to the sum $Q_1 + Q_2$. One can think of this flame as converting A to B by reaction (i), and B thereupon being almost immediately converted to P by a faster reaction (ii).

We again define functions $H_i(T)$ according to (19), with $\bar{c}$ given by (20). We assume that T_- , T_1 , T_2 , and T_+ are all of the same order of magnitude, and $T_1 - T_-$, $T_2 - T_-$, $T_+ - T_1$, $T_+ - T_2$, all are $O(1)$ quantities. The temperature scale is adjusted so that $T_+ - T_- = 1$.

We consider the consequences of various inequalities involving the functions H_i . When such an inequality is written, it will be assumed that the difference of the two quantities concerned is $O(1)$. This is the typical case, because the range of at least one of the functions H_i is of order unity.

Immediate consequences of Sec. 2 are:

- 1) If $H_2(T_1) < H_1(T_1)$, then F1 is realizable.
- 2) If $H_1(T_2) < H_2(T_2)$, then F2 is.

The next structures to be considered are possible combinations of 2 flames. Note, from (16) and the fact that $M \sim \eta^{1/2}$, that the mass flux for F1 is

$$M_1 = C_1 H_1 c_1^2 \exp(-E_1/T_1) \quad , \quad (35)$$

where

$$\varepsilon_1 = T_1^2/E_1 \quad ,$$

and C_1 is some constant, $C_1 = O(1)$. Hence,

$$\bar{\varepsilon} \ln M_1 = \bar{\varepsilon}(\ln B_1 - E_1/T_1 + 2 \ln \varepsilon_1) + O(\bar{\varepsilon}) \quad .$$

$$\text{But } |\ln \varepsilon_1| = \ln \frac{1}{\varepsilon_1} \leq \ln 1/\bar{\varepsilon}$$

$$\bar{\varepsilon} \ln M_1 = H_1(T_1) + O(\bar{\varepsilon} \ln 1/\bar{\varepsilon}) \quad .$$

In a similar manner,

$$\bar{\varepsilon} \ln M_2 = H_2(T_2) + o(1) \quad ,$$

$$\bar{\varepsilon} \ln M_{1+} = H_2(T_+) + o(1) \quad ,$$

$$\bar{\varepsilon} \ln M_{2+} = H_1(T_+) + o(1) \quad .$$

It turns out that the mass fluxes of these four simple flames are ordered in the same way as their velocities. Thus, for example, if $H_2(T_+) < H_1(T_1)$, then F12, built on the products of F1, is slower than F1 itself, and so one can conceive of the two flames both existing, but the distance between them ever increasing. The flame F1 precedes, and is faster than, F12. We call this total configuration F1,12:

3) If $H_2(T_+) < H_1(T_1)$, then F1,12 is realizable.

Similarly:

4) If $H_1(T_+) < H_2(T_2)$, then F2,12 is.

The most interesting flames, however, are seen when neither 3) nor 4) hold. This last case is split into two subcases: $H_1(T_1) < H_2(T_+) < H_1(T_+)$, and $H_2(T_2) < H_1(T_+) < H_2(T_+)$. It can be easily checked that these two are exclusive and, excluding cases when equality holds somewhere, exhaust the complement of 3) and 4). Since 3) and 4) do not hold, the diverging configurations F1,12 and F2,21 are not possible. Indeed if such a combination of flames like F1,12 existed at one time, then the rear flame F12 would approach the forward flames F1. As it does so, its effect is to heat up the forward one. As this happens, the speed of the forward increases (this is feasible because our expression for M , as in (35), is an increasing function of T). The question now is whether this heating from the rear is sufficient to raise the velocity of the forward part to equal that of the trailing F12. Of course, the temperature of F1 cannot by this mechanism be raised above T_+ , which is the temperature of F12. And it seems reasonable that the equality of speeds will be attained at a temperature T_0 such that $H_1(T_0) = H_2(T_+)$. Therefore our conjecture (to be verified) is that such a tandem configuration, with F1 (ahead) and F12 (behind) traveling at a fixed distance apart, is realizable if there is a T_0 satisfying the above equation. But this is true precisely in the first subcase. We call this tandem flame F1-12.

5) If $H_1(T_1) < H_2(T_+) < H_1(T_+)$, then F1-12 is realizable.

Similarly,

6) If $H_2(T_2) < H_1(T_+) < H_2(T_+)$, then F2-21 is realizable.

It should again be emphasized that at this point, (5) and (6) are just conjectures. However, they can be verified in the following manner. If a tandem structure exists, it should correspond to the solution of a reduced

problem in the spirit of (9), and this reduced problem should be uniquely solvable.

This is, in fact, the case. For F1-12, for example, the reduced problem takes the form

$$D\ddot{U} - \bar{M}\dot{U} = 0 \quad , \quad \bar{x} \neq 0 \quad , \quad \bar{x} \neq 2 \quad ;$$

$$U(\pm\infty) = U_{\pm} \quad ,$$

$$[D\dot{U}]_{0-}^{0+} = -\beta_1 K_1 \quad , \quad [D\dot{U}]_{2-}^{2+} = -\beta_2 K \quad .$$

Here β_2 , $U_{\pm}$, and $T(0) = T_0$ constitute the given data; the problem is then to determine β_1 , ℓ , and $U(\bar{x})$. The problem has a unique solution. The constant β_2 is known by a layer analysis very like that in Sec. 2. However, the coefficient β_1 should also be involved with a layer analysis. And indeed such an analysis can be performed; it yields a functional relation

$$\beta_1 = F(r, \dot{U}(0+)) \quad ,$$

where r is given by (24) with T_+ in the denominator replaced by T_0 . This relation can be inverted to yield

$$r = R(\beta_1, \dot{U}(0+)) \quad . \quad (36)$$

The proper consistency check on the above reduced problem, then, is (1) solve it, and find β_1 and $\dot{U}(0+)$; (2) determine r from (36); (3) if this r satisfies (24) (T_+ in denominator replaced by T_0). We rewrite (24) in the form

$$\ell \ln r = H_2(T_+) - H_1(T_0) \quad . \quad (37)$$

Now T_0 was chosen to make the right side vanish; but if we now reason that this is only the first approximation to the true value of T_0 , then (37) can be used to obtain a corrected value for T_0 . Since $H_1'(T_0) = O(1)$, and $r = O(1)$, it turns out that the correction will only be $O(\bar{\epsilon})$, so the original value of T_0 will be correct within our general range of accuracy. The details of the tandem analysis can be found in [3].

In summary, the possibility of the various flame types 1,2, etc., can be found by testing each of the cases 1) - 6) in turn. Cases 3) - 6) are mutually exclusive, but any of the latter could hold in conjunction with 1) or 2). There result nonunique flame structures; which one is realized in a given observation would depend on how and to what extent the gas mixture is ignited. A case of nonuniqueness is the case when $T_1 < T_2$, and

$$H_2(T_1) - H_1(T_1) < H_1(T_2) - H_2(T_2) < H_2(T_+) - H_1(T_+) .$$

In this case, types 1, 2, and 1-12 are all realizable.

4. Reactions in Parallel

The combustion process now allows the reactant A to be consumed in two competing fashions:

Again, each reaction is exothermic with high activation energy, and the unburned state $U(-\infty) = U_- = \begin{bmatrix} T_- \\ Y_- \end{bmatrix}$ is prescribed (here Y represents the dimensionless concentration of A).

There are only two conceivable simple flames: F1 and F2, with final temperatures $T_1 = T_- + Q_1 Y_-$ and $T_2 = T_- + Q_2 Y_-$, respectively. For the sake of definiteness, we assume $Q_1 < Q_2$, hence

$$T_1 < T_2 .$$

Temperature is scaled so that $T_2 - T_- = 1$. Assume $T_2 - T_1, T_1 - T_- = O(1)$. We define H_i again by (19) and (20) with T_+ replaced by T_2 . According to the criterion in Sec. 2, F1 is realizable if $H_1(T_1) > H_2(T_1)$, and F2 is if $H_2(T_2) > H_1(T_2)$. Four cases therefore arise:

- (a) $H_1(T_i) < H_2(T_i), i = 1, 2$,
- (b) $H_1(T_i) > H_2(T_i), i = 1, 2$,
- (c) $H_1(T_1) > H_2(T_1), H_1(T_2) < H_2(T_2)$,
- (d) $H_1(T_1) < H_2(T_1), H_1(T_2) > H_2(T_2)$.

The cases are depicted by these four sample graphs of functions H_i (dotted lines represent $H_1(T)$, dashed lines $H_2(T)$).

In case (a), only F2 is possible; in case (b), only F1; in case (c), either F1 or F2, and in case (d), neither F1 nor F2. This suggests there

may be an interactive, nonsimple, flame type in case (d), since neither simple flame can exist. The only way both reactions can be significant in the burning process is for their H 's to be the same. It is clear from the graph that this occurs at a value T_o (T_1, T_2). We therefore postulate a flame burning at temperature T_o in which both reactions take part. This situation can be fit into the framework of Case II in Sec. 3. Such a flame would be governed by (17) with $U = \begin{bmatrix} T_o \\ Y \end{bmatrix}$. The reduced problem would be (33,32). More specifically variant (A) of that problem applies, since

$$U_+ = \begin{bmatrix} T_o \\ 0 \end{bmatrix} \text{ is given.}$$

We now indicate the solution of that problem. First, it is clear that for some $\theta \in (0,1)$, T_o may be represented as $T_o = \theta T_1 + (1 - \theta) T_2$. Hence $T_o - T_- = \theta Y_- Q_1 + (1-\theta) Y_- Q_2$ and since $K_i = \begin{bmatrix} Q_i \\ -1 \end{bmatrix}$, we have

$$U_+ - U_- = \alpha_1 K_1 + \alpha_2 K_2 ,$$

where $\alpha_1 = \theta Y_-$, $\alpha_2 = (1-\theta) Y_-$. The ratio r is now determined from (34), and hence $\bar{M} = a_1/\alpha_1$, and the profile $U(\bar{x})$ from (33a).

The consistency check now requires (24) to hold with T_+ replaced by T_o . This equation can be written

$$\bar{\epsilon} \ln r = H_2(T_o) - H_1(T_o) . \quad (38)$$

Since T_o was chosen so the right side vanishes, there appears to be an inconsistency. But the inconsistency is only superficial; the equation (38) simply says that the previous value of T_o should be adjusted (by an amount $O(\bar{\epsilon})$) to obtain a more accurate value.

It should be remarked that the "mixed" flame constructed in case (d) apparently also exists in case (c), because again, H_i have a common value at T_o . But in that case, the mixed flame is unstable in a certain sense: if its temperature is perturbed by a small amount, it will evolve into one of the two simple flames. In case (d), this instability does not occur.

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