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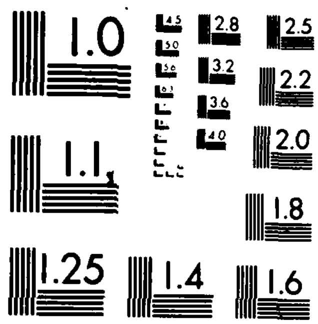

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LECTURE ON MATHEMATICAL COMBUSTION

Lecture 3: General Deflagrations

Technical Report No. 148

J.D. Buckmaster & G.S.S. Ludford

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Theoretical and Applied Mechanics

Thurston Hall
Ithaca, New York

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Lecture 3

GENERAL DEFLAGRATIONS

In the last lecture we examined the plane, steady, adiabatic, premixed flame and deduced an explicit formula for its speed. By using a judicious choice of parameters this formula can be made to agree roughly with experiment; precision is not a reasonable goal, given the crude nature of our model. Noteworthy is the extreme sensitivity of the speed to variations in the flame temperature: an $O(1)$ change generates an exponentially large change in flame speed. Such variations in speed (caused, for example, by changes in mixture strength) are not excessive numerically (at least for fuels burnt in air), because activation energies and fractional changes in temperature are modest; but in an asymptotic analysis they present a potential obstacle to discussion of multidimensional and/or unsteady flames. Then significant variations, spatial and/or temporal, in the flame temperature can be expected and, if the sensitivity mentioned above is any guide, there will be correspondingly large spatial and/or temporal variations in the flame speed. A mathematical framework in which to accommodate these is not obvious. (The first lecture dealt with special circumstances for which such variations were manageable.)

As a consequence, attempts to discuss general deflagrations have, for the most part, been limited to situations where there is an <u>a priori</u> guarantee that variations in the flame temperature are $O(\theta^{-1})$; then flame-speed changes are $O(1)$ and present no mathematical difficulties. Two approaches are known to provide the guarantee and this lecture is largely devoted to their disclosure.

1. The Hydrodynamic Limit

At the end of section 2.4 the steady plane deflagration was found to have a thickness $5\lambda/c_p M_r$, and this may be taken as the nominal thickness of a general deflagration. We start by restricting attention to waves whose characteristic length (e.g. minimum radius of curvature) is large compared to their nominal thickness. On this length scale, such a wave is simply a surface across which jumps in temperature and density occur subject to Charles's law (as in appropriate for an essentially isobaric process).

If the ratio of the two scales is ε, then on either side of the surface the appropriate variables are

$$(\bar{x},\bar{y},\bar{z},\bar{t}) = \varepsilon(x,y,z,t); \tag{1}$$

so that the governing equations (2.18b,19,20) becomes

$$\partial\rho/\partial\bar{t} + \bar{\nabla}\cdot(\rho \mathbf{v}) = 0,\ \rho D\mathbf{v}/D\bar{t} = -\bar{\nabla}p + \varepsilon P[\bar{\nabla}^2\mathbf{v} + \frac{1}{3}\bar{\nabla}(\bar{\nabla}\cdot\mathbf{v})], \tag{2}$$

$$\rho DT/D\bar{t} - \varepsilon\bar{\nabla}^2 T = 0,\quad \rho DY/D\bar{t} - \varepsilon L^{-1}\bar{\nabla}^2 Y = 0 \tag{3}$$

(We have not written the equations for components other than the single reactants $i = 1$, and the subscript 1 has been dropped.) As $\varepsilon \to 0$, we have

$$DT/D\bar{t} = DY/D\bar{t} = 0, \tag{4}$$

i.e. constant values of T and Y are carried by the fluid particles. We conclude that

$$T = T_f,\quad Y = Y_f \tag{5}$$

everywhere ahead of the discontinuity surface if, as we shall suppose, these constant values are assumed by each particle at its point of origin. Likewise

$$T = T_b, \quad Y = 0 \tag{6}$$

everywhere behind the discontinuity since, as we shall see presently, these values are assumed by each particle as it leaves the flame. Charles's law (2.18a) now shows that ρ has the constant values $\rho_f, \rho_b = \rho_f/\sigma$ on the two sides of the discontinuity, where

$$\sigma = \rho_f/\rho_b = T_b/T_f = 1 + Y_f/T_f \tag{7}$$

is the expansion ratio due to the flame. We are left the Euler's equations

$$\bar{\nabla}\cdot\mathbf{v} = 0, \quad \rho D\mathbf{v}/\partial\bar{t} = -\bar{\nabla}p \tag{8}$$

for an incompressible, ideal fluid, i.e. one devoid of both viscosity and heat conduction.

The two ideal-fluid regions are coupled through the jump conditions

$$\rho_f(v_{nf}+V) = \rho_b(v_{nb}+V), \quad \mathbf{v}_{\perp f} = \mathbf{v}_{\perp b}, \tag{9}$$

$$p_f+\rho_f(v_{nf}+V)^2 = p_b+\rho_b(v_{nb}+V)^2, \quad T_f+Y_f = T_b; \tag{10}$$

here V is the speed of the deflagration wave back along its normal (figure 1), and the subscript "$\perp$" denotes the component perpendicular to $\mathbf{n}$, i.e. in the tangent plane. These conditions are derived in the same way as for a shock wave in reactionless gasdynamics, i.e. by integrating the basic equations (2.18b,19,20) through the flame. Indeed, the conditions (9) and (10a) are identical to those for a shock since they follow from the same continuity and momentum equations. The requirement (10b) can also be recognized as a Rankine-Hugoniot condition, but with kinetic energy neglected and a heat-release term (Y_f) added. It follows from the combination

$$\rho D(T+Y)/Dt = \nabla^2(T+L^{-1}Y) \qquad (11)$$

of the basic equations (2.20).

As for the shock wave, these jump conditions are insufficient. If the state f immediately ahead of the wave is given, there are five scalar equations for the six unknown scalars ρ_b $(=\rho_f T_f/T_b)$, v_{nb}, $v_{\perp b}$, p_b, and V. In the case of a shock, another condition is imposed from outside (such as the deflection of the streamlines at a sharp body or the pressure p_b behind the wave in a shock tube). Here there is no external condition; the deficiency arises from discarding information by using only the combination (11) of the basic equations (2.20). The reaction rate then plays no role in the derivation of the jump conditions. Otherwise stated, the combustion inside the wave will provide information about the burning rate $\rho_f W$, i.e. the wave speed

$$W = v_{nf} + V. \qquad (12)$$

Evaluation of W from a combustion analysis has often been side-stepped, even though it should be considered the central question of premixed flames. Instead, hypotheses are introduced; the simplest is that W is a constant, given by the burning-rate formula (2.43) of steady, plane deflagrations. This hypothesis is justified for slowly varying flames (section 3) when $L = 1$, and we shall use it in lecture 10. But, in general, it is not acceptable and attempts have been made (notably by Markstein) to modify it, in particular by taking into account non-planar characteristics of the flame.

The remainder of this lecture will be preparation for the more general combustion analysis that follows in the next.

2. Governing Equations for the Constant-Density Approximation

Although the formulation can be carried through for the full equations (2.18-20), all the essential features are preserved under the assumption that density variations due to the presence of the flame are negligible.' If no temperature differences are imposed on the flow, the velocity field is that of a constant-density fluid and can be calculated in advance; we shall suppose the fluid is at rest. In other words, we shall set

$$\rho = 1, \quad \underset{\sim}{v} = 0 \tag{13}$$

in the full equations to obtain

$$\partial T/\partial t - \nabla^2 T = \Omega - \theta^{-1}\psi(T), \quad \partial Y/\partial t - \mathcal{L}^{-1}\nabla^2 Y = -\Omega \tag{14}$$

as those governing the combustion field under the constant-density approximation. (All equations (2.20b) except the first, corresponding to the single reactant, can be omitted; the subscript 1 can then be dropped.) Note that we have added a term $-\theta^{-1}\psi(T)$ to the temperature equation, representing small bulk heat loss.

If the representative mass flux M_r is chosen to be the burning rate (2.43) of the plane, steady (adiabatic) deflagration, then the reaction term becomes

$$\Omega = \mathcal{D} Y e^{-\theta/T} \text{ with } \mathcal{D} = Y_f^2 \theta^2 e^{\theta/T_b} / 2\mathcal{L} T_b^4. \tag{15}$$

Note that $\mathcal{L}$ is not necessarily equal to 1 in these equations: the Lewis number plays a very important role in the analysis, especially for unsteady flames. Finally, the heat-loss term is difficult to justify in a multidimensional context (radiation loss, one of the few legitimate candidates, is negligibly small unless there are solid particles such as soot in the mixture); but for quasi-plane flames it can represent multidimensional effects such as losses to sidewalls.

We shall require that

$$T \to T_f, \quad Y \to Y_f \quad \text{as} \quad x \to -\infty \tag{16}$$

and deal exclusively with situations where equilibrium prevails behind the flame sheet, i.e.

$$Y = 0 \quad \text{in the burnt gas} \tag{17}$$

The temperature behind the flame will be close to the adiabatic flame temperature (2.29).

The constant-density approximation, on which most of the premixed flame analysis in these lectures is based, clearly provides substantial simplifications. It can be justified as a formal limit in which the heat released by the reaction becomes vanishingly small (compared to the existing thermal energy of the mixture). Small heat release can be due to either a scarcity of reactant $(Y_f \to 0)$ or weak combustion $(T_f \to \infty)$; by confining ourselves to dilute mixtures, we have already assumed the former. The relevant parameter is the expansion ratio (7); asymptotic expansions in $\sigma-1$ provide a formal basis for the approximation.

3. Slow Variations with Loss of Heat

As an introduction to the more complicated analysis of multidimensional flames consider first a plane flame sheet (figure 1), looking like the adiabatic deflagration studied in section 2.4 but moving unsteadily because of local fluctuations in T and Y (represented by the time derivatives). In general, the flame speed can be defined in terms of the mass flux of the mixture through the sheet. (This is a well-defined concept in the limit $\theta \to \infty$; for θ finite there is no natural definition, except when the combustion field is steady in some moving frame.) For the constant-density approximation adopted here, the speed is just

$$V = -\dot{x}_*(t).$$

Note that, since the speed is not defined for finite θ, to expand it in the subsequent asymptotic analysis would be a futile gesture.

Suppose now that changes in the flame speed occur on an $O(\theta)$ time scale, i.e. that

$$\tau = t/\theta \qquad (19$$

is the appropriate (slow) time variable to describe them. Then, for an ob moving with the flame sheet, the combustion field is quasi-steady to leading order (i.e. steady for $t = O(1)$). The temporal variations, along with heat loss, create $O(\theta^{-1})$ perturbations, and hence generate only $O(\theta^{-1})$ variations in the flame temperature.

When the coordinate

$$n = x - x_*(t), \qquad (20)$$

based on the flame sheet, is introduced the basic equations (14) become

$$\theta^{-1}\partial T/\partial\tau + V\,\partial T/\partial n - \partial^2 T/\partial n^2 + \theta^{-1}\psi = -\theta^{-1}\partial Y/\partial\tau - V\partial Y/\partial n + L^{-1}\partial^2 Y/\partial n^2 = \Omega. \qquad (21)$$

These govern the motion of what is known as a slowly varying flam (SVF). To integrate the equations it is first necessary to say something about the flame temperature. To leading order, we have

$$V\partial(T+Y)/\partial n = \partial^2(T+L^{-1}Y)/\partial n^2 \qquad (22)$$

everywhere; so that, on integrating from $n = -\infty$ to $0+$ and using the boundary conditions (16,17), we have

$$V(T_* - T_f - Y_f) = \partial T/\partial n|_{0+}, \tag{23}$$

where T_* is the leading-order temperature at the flame. Since the derivative vanishes (as will be seen immediately), we conclude that

$$T_* = T_b, \tag{24}$$

the adiabatic flame temperature (2.29).

In view of the requirements (16,17) the solution of equations (21) in the frozen region ahead of the flame sheet is

$$T = T_f + Y_f e^{Vn}, \quad Y = Y_f(1-e^{LVn}) \text{ for } n < 0, \tag{25}$$

correct to leading order. To the same order behind the flame sheet, T is constant (hence showing that the derivative in the result (23) is zero, as anticipated); to one more term we find

$$T = T_b - \theta^{-1}[V^{-1}\psi(T_b)n + T_b^2\phi_*(\tau)], \quad Y = 0 \quad \text{for } n > 0 \tag{26}$$

by writing $T = T_b$ in the θ^{-1} terms of the temperature equation. Here ϕ_*, representing the perturbed flame temperature, is as yet unknown.

The structure problem for the reaction zone determines ϕ_* as a function of V. This problem has already been discussed in section 2.5, where the expression (2.47) for the temperature gradient just ahead of the flame sheet was developed. The same gradient can be calculated from the result (25a), leading to the relation

$$V = e^{-\phi_*/2}. \tag{27}$$

Clearly, there is the same temperature sensitivity as for steady adiabatic deflagrations, as expected. Moreover, for such a deflagration the perturbation ϕ_* vanishes and $V = 1$, which confirms the burning-rate formula (2.43).

Another relation between ϕ_* and V comes from calculating the change in enthalpy of the mixture between its fresh and burnt states. For that purpose, we rewrite equation (22) correct to $O(\theta^{-1})$ before integrating it as before, to obtain

$$\theta^{-1}\int_{-\infty}^{0+} \frac{\partial}{\partial\tau}(T+Y)dn + [V(T+Y)]_{-\infty}^{0+} + \theta^{-1}\int_{-\infty}^{0+} \psi dn = [\frac{\partial T}{\partial n} + L^{-1}\frac{\partial Y}{\partial n}]_{-\infty}^{0+} . \quad (28)$$

The integrals can be evaluated to leading order by means of the formulas (25); we find

$$\int_{-\infty}^{0+} \frac{\partial}{\partial\tau}[Y_f(e^{Vn}-e^{LVn})]dn = Y_f\dot{V}\int_{-\infty}^{0+} n(e^{Vn}-e^{LVn})dn = -Y_f(1-L^{-1})V^{-2}\dot{V},$$

$$\int_{-\infty}^{0+} \psi(T_f+Y_f e^{Vn})dn = [\int_0^{\infty}\psi(T_f+Y_f e^{-\nu})d\nu]V^{-1},$$

where the dot is used to signify rate of change on the τ-scale. The formulas (26) and boundary conditions (16) enable the remaing terms to be calculated; we have

$$[V(T+Y)]_{-\infty}^{0+} = V(T_*-T_b) = -\theta^{-1}T_b^2V\phi_*,$$

$$[\partial T/\partial n]_{-\infty}^{0+} = -\theta^{-1}\psi(T_b)V^{-1}, \quad [\partial Y/\partial n]_{-\infty}^{0+} = 0.$$

The equation (28), in which all terms have now been evaluated to $O(\theta^{-1})$, therefore gives

$$\phi_* = \Psi V^{-2} - bV^{-3}\dot{V} \quad \text{with} \quad b = Y_f(1-L^{-1})/T_b^2; \quad (29)$$

here

$$\Psi = [\psi(T_b) + \int_0^\infty \psi(T_f+T_f e^{-\nu})d\nu]/T_b^2, \tag{30}$$

the two terms representing heat lost to the burnt mixture and through the sidewalls ahead of the flame sheet, respectively.

By eliminating ϕ_* between the two relations (27) and (29), we obtain an equation for V, namely

$$b\dot{V} = V^3 \ln V^2 + \Psi V. \tag{31}$$

The only difference when the constant-density approximation is not used is a more complicated formula for b. The crucial property

$$b \lessgtr 0 \text{ accordingly as } l \lessgtr 1 \tag{32}$$

is unaffected, however. Note that the SVF is not a solution of the general initial-value problem (only the value of V may be prescribed at $\tau = 0$); it merely describes the subsequent behavior of any flame that survives development on the t-scale. Thus, a prediction of instability is reliable but not one of stability, since the flame may have already lost stability during its evolution on the t-scale.

Consider first the steady state (figure 2) determined by setting $\dot{V} = 0$ in the evolution equation (31), i.e.

$$V = 0 \text{ or } V^2 \ln V^2 + \Psi = 0. \tag{33}$$

On the first of these $\phi_* = +\infty$, so that the perturbation analysis breaks down; the corresponding nonuniformity has never been treated. The second curve provides two solution branches so long as the heat loss is not too large, i.e. Ψ is less than e^{-1} (= 0.368); the adiabatic flame speed $V = 1$ is attained on the upper branch as $\Psi \to 0$, so that it is plausible to suppose that this is the physically relevant one. No solution exists for $\Psi > e^{-1}$: steady combustion cannot be sustained if the heat loss is too large, any existing flame being quenched. It is interesting that the speed of the flame at quenching, namely $e^{-\frac{1}{2}}$ (= 0.607) times its adiabatic value, is completely independent of the nature of the heat loss, i.e. the form of the function ψ. The quenching phenomenon provides a qualitative explanation of the Davy safety lamp: the wire gauze surrounding the flame is an effective heat sink, preventing the propagation of the flame beyond its confines.

Equation (31) describes the evolution of plane SVFs. When $L = 1$, b is zero and there is no evolution: equidiffusion prevents any variation on the τ-scale. In fact, since the equation is asymptotic, there is no evolution when L is close to 1, i.e.

$$L^{-1} = 1-\ell/\theta \quad \text{with } \ell = O(1). \tag{34}$$

But then a treatment on the t-scale is possible in certain circumstances, leading to the near-equidiffusion flame (NEF) discussed later.

An immediate consequence of the evolution for $L > 1$ $(b > 0)$ is that the flame is unstable: any deviation of V from its value on the upper branch of the curve in figure 2 is amplified. The same conclusion cannot be drawn for $L < 1$, but this is a consequence of considering planar disturbances only. Lecture 5 will examine the linear stability of plane deflagration waves in complete detail, and find that plane SVFs are unstable to non-planar disturbances for $L > 1$. Thus, the SVFs are unstable for all values of L, which decreases their value as a class of solutions (but does not eliminate them).

4. Multidimensional Flames

Consider now situations in which the flame sheet, in addition to being unsteady, moves in a non-planar fashion. The goal is to find conditions under which the variations in flame temperature, both temporal and spatial, are $O(\theta^{-1})$ at most. To that end we shall perform an integration of the basic equations (14) that is a generalization of the one done on their plane version (21) in the last section.

The x-axis is taken instantaneously along the normal to the flame sheet at the point of interest (pointing into the burnt gas), and a new variable

$$n = x - F(0,0,t) \tag{35}$$

is introduced, as for plane sheets (cf. equation (20)); here $F(y,z,t)$ denotes the position of the sheet. Equations (14) then become

$$\partial T/\partial t + V\partial T/\partial n - \partial^2 T/\partial n^2 - \nabla_\perp^2 T + \theta^{-1}\psi(T) = -\partial Y/\partial t - V\partial Y/\partial n - L^{-1}\partial^2 Y/\partial n^2 - L^{-1}\nabla_\perp^2 Y = \Omega \tag{36}$$

where

$$V = -\dot{F}(0,0,t) \tag{37}$$

is the speed of the sheet back along its normal at the instant considered and, as in section 1, the subscript "$\perp$" denotes the component perpendicular to x.

Equation (36a) is now integrated with respect to n from $-\infty$ to $0+$, thereby yielding

$$\int_{-\infty}^{0+} \frac{\partial}{\partial t}(T+Y)dn + [V(T+Y)]_{-\infty}^{0} + \theta^{-1}\int_{-\infty}^{0+}\psi\, dn =$$

$$\left[\frac{\partial T}{\partial n} + L^{-1}\frac{\partial Y}{\partial n}\right]_{-\infty}^{0+} + \int_{-\infty}^{0+}\nabla_\perp^2(T+L^{-1}Y)dn, \tag{38}$$

which should be compared to equation (28). Certain terms can be evaluated almost as there; thus,

$$[V(T+Y)]_{-\infty}^{0+} = V(T_*-T_b),\ [\partial T/\partial n]_{-\infty}^{0+} = \partial T/\partial n\Big|_{0+},\ [\partial Y/\partial n]_{-\infty}^{0+} = 0,$$

so that we may write

$$V(T_*-T_b) = \frac{\partial T}{\partial n}\Big|_{0+} + \int_{-\infty}^{0+} [\nabla_\perp^2(T+L^{-1}Y) - \frac{\partial H}{\partial t}]dn - \theta^{-1}\int_{-\infty}^{0+} \psi dn. \qquad (39)$$

This expresses the deviation of the flame temperature T_* from its adiabatic value T_b in terms of the heat lost to the burnt mixture, the transverse diffusion of heat and reactant up to the flame sheet, the temporal variations in enthalpy H of the mixture ahead of the flame sheet, and the heat loss up to the flame sheet.

If deviations of T_* from T_b are to be $O(\theta^{-1})$, the right side of equation (39) must be of the same order. This is guaranteed when the terms in $\partial/\partial n$, $\nabla_\perp^2$, and $\partial/\partial t$ are made separately small, a step that can be taken in two different ways. One way is to confine attention to disturbances of a steady, plane deflagration that vary over times and distances $O(\theta)$. These SVFs are a generalization of the ones introduced in the last section, where only temporal variations were considered. The second way is suggested by the ineffectiveness of the SVF analysis for L close to 1. In the distinguished limit (34), equation (36a) becomes

$$\partial H/\partial t + V\partial H/\partial n-(\partial^2\partial n^2+\nabla_\perp^2)H = \theta^{-1}[\ell(\partial^2/\partial n^2+\nabla_\perp^2)Y-\psi(T)], \qquad (40)$$

of which

$$H = H_f + O(\theta^{-1}) \text{ (everywhere)} \qquad (41)$$

is one solution. For the corresponding class of solutions, called near-equidiffusion flames (NEFs),

$$\frac{\partial T}{\partial n}\Big|_{0+} = \frac{\partial H}{\partial n}\Big|_{0+},\ \nabla_\perp^2(T+L^{-1}Y) = \nabla_\perp^2 H+O(\theta^{-1}),\ \frac{\partial H}{\partial t} \qquad (42)$$

are all $O(\theta^{-1})$, so that the right side of equation (38) is of that order.

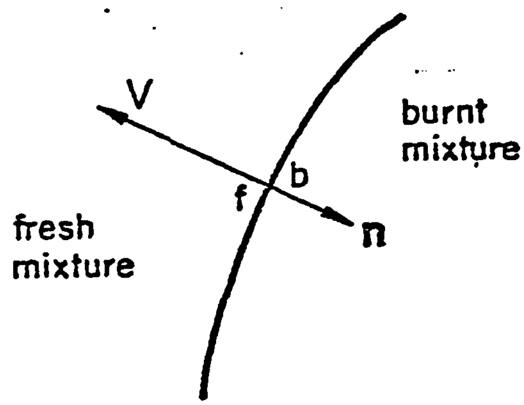
It should be emphasized that SVFs and NEFs are restricted classes of solutions, identified by setting down sufficient (but not necessary) conditions for the flame-temperature variations to be $O(\theta^{-1})$, itself a sufficient condition for the efficacy of our asymptotic method. While these classes may be the only general ones, special circumstances make it possible to treat other premixed flames. Lack of time prevents our discussing the most important of these, namely the spherical (premixed) flame: symmetry ensures that the temperature does not vary at all over its flame sheet, so that it need not be either an SVF or an NEF. (Nevertheless, for certain parameter values it is an SVF and for others an NEF.)

In the next lecture, the equations governing the SVF and the NEF will be derived and then solved for a basic non-uniform velocity field: stagnation-point flow.

Figure Captions

3.1 Notation for flame as hydrodynamic discontinuity.

3.2 Steady flame speed V versus heat-loss parameter Ψ . Arrows show direction in which speed changes for $L > 1$.



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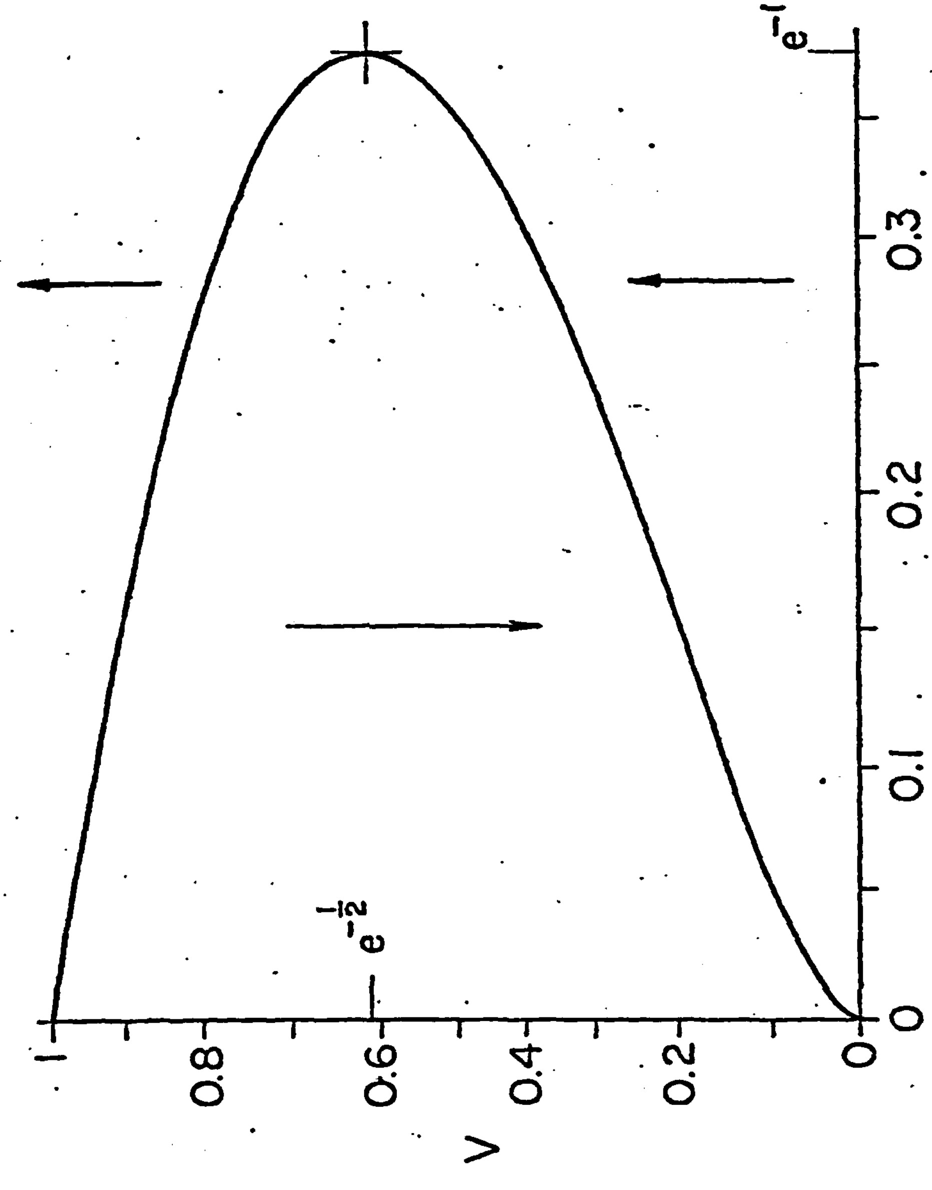
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

In the last lecture we examined the plane, steady, adiabatic, premixed flame and deduced an explicit formula for its speed. By using judicious choice of parameters this formula can be made to agree roughly with experiment; precision is not a reasonable goal, given the crude nature of our model. Noteworthy is the extreme sensitivity of the speed to variaitons in the flame temperature: an O(1) change generates an exponentially large change in

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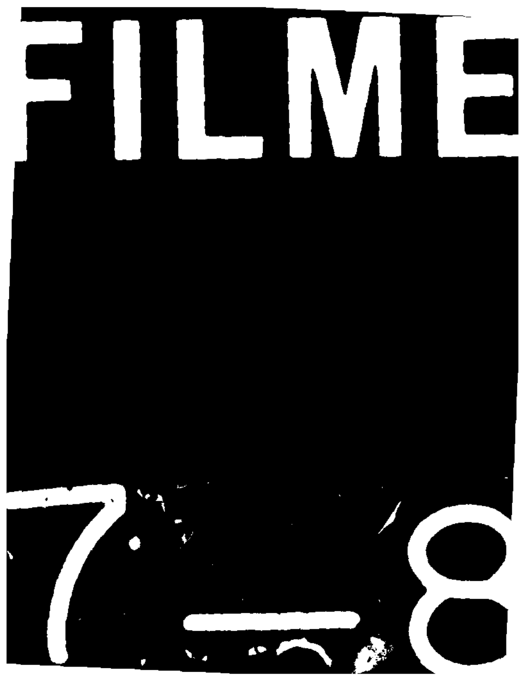
SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) flame speed. Such variations in speed (caused, for example, by changes in mixture strength) are not excessive numerically (at least for fuels burnt in air), because activation energies and fractional changes in temperature are modest; but in an asymptotic analysis they present a potential obstacle to discussion of multidimensional and/or unsteady flames. Then significant variations, spatial and/or temporal, in the flame temperature can be expected and, if the sensitivity mentioned above is any guide, there will be correspondingly large spatial and/or temporal variations in the flame speed. A mathematical framework in which to accomodate these is not obvious. (The first lecture dealt with special circumstances for which such variations were manageable.)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