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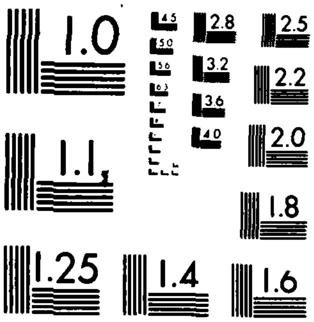

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LECTURES ON MATHEMATICAL COMBUSTION

Lecture 2: Governing Equations, Asymptotics, and Deflagrations

Technical Report No. 147

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

January 1983

Theoretical and Applied Mechanics

Thurston Hall
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U.S. Army Research Office
Research Triangle Park, NC 27709

Contract No. DAAG29-81-K-0127

Cornell University
Ithaca, NY 14853

Contents

A

Lecture 2

GOVERNING EQUATIONS, ASYMPTOTICS, AND DEFLAGRATIONS

The problem of formulating the governing equations of combustion consists, at its simplest, in characterizing the flow of a viscous, heat-conducting mixture of diffusing, reacting gases. This is a formidable task that could fill a week of lectures by itself, most of which would not be of great interest to a mathematical audience. Mindful of this, we shall limit ourselves to a description, rather than a derivation, of the simplest equations that can be brought to bear on combustion problems. Only the most important assumptions normally used to justify the equations will be discussed; for a more extensive treatment the reader is referred to Buckmaster & Ludford (1982, ch.1)

We shall then outline the asymptotic method on which the whole theory rests and use it to solve the basic problem of combustion: the steady propagation of a plane deflagration wave.

1. Equations for Dilute Mixtures

The easiest framework in which to understand the field equations is the "reactant bath". We suppose that most of the mixture consists of a single inert component (e.g. nitrogen), the properties of which determine those of the mixture (e.g. viscosity, specific heat). The reacting components (and their products) are highly diluted by immersion in this bath of inert.

Mass concentration for the mixture is always described by the single-fluid equation

$$\partial\rho/\partial t + \nabla\cdot(\rho \mathbf{v}) = 0, \qquad (1)$$

where ρ is the density and $\underset{\sim}{v}$ the velocity. But only for dilute mixtures is the overall momentum balance identical to that for a single homogeneous fluid, namely

$$\rho\, D\underset{\sim}{v}/Dt = \underset{\sim}{\nabla}\cdot\underset{\approx}{\Sigma}, \tag{2}$$

where

$$\underset{\approx}{\Sigma} = -(p + \tfrac{2}{3}\kappa\underset{\sim}{\nabla}\cdot\underset{\sim}{v})\underset{\approx}{I} + \kappa[\underset{\sim}{\nabla}\underset{\sim}{v}+(\underset{\sim}{\nabla}\underset{\sim}{v})^{T}] \tag{3}$$

and p is pressure; bulk viscosity has been neglected.

A single-fluid equation for energy balance is also justified, provided account is taken of the release of heat by chemical reaction. But here additional approximations are made, based on the observation that temperatures are high and gas speeds low for a large class of combustion phenomena (excluding detonation); more precisely, a characteristic Mach number is small (typically in the range 10^{-2}-10^{-3}). Then the only significant form of energy, other than that of chemical bonding, is thermal; kinetic energy makes a negligible contribution to the energy balance. For the same reason, the conversion of kinetic energy into thermal energy by way of viscous dissipation can be ignored. Thus, when variations of the specific heat c_p with temperature are neglected, we have

$$\rho\, c_p DT/Dt - \underset{\sim}{\nabla}\cdot(\lambda\underset{\sim}{\nabla}T)-\partial p/\partial t = q, \tag{4}$$

where q is the heat released per unit volume of the fluid by chemical reaction; the form of q is considered later.

In addition, the assumption of small Mach number implies that spatial variations in pressure are small, so that $\partial p/\partial t$ in the energy balance (4) is due to imposed, uniform pressure variations. We shall assume that the imposed pressure is constant, i.e. the term vanishes. The pressure term in the momentum equation (2) cannot be neglected, however; the small spatial variations are needed to account for changes in the weak velocity field. A further consequence of the virtual constancy of the pressure is that the equation of state of the mixture is Charles's law

$$\rho T = mp_c/R \tag{5}$$

if the inert is a perfect gas. Here m is the molecular mass of the inert, p_c the imposed constant pressure, and R the gas constant.

Consider now the individual components of the mixture, denoting the density of the i-component by ρY_i, where Y_i is the mass fraction and $i = 1,2,\ldots,N$. The reactants and their products are convected with the gas speed $\underset{\sim}{v}$, diffuse relative to the inert diluent, and are consumed or generated by reaction. The diffusion laws of general mixtures are complicated, involving a diffusion matrix; but for dilute mixtures the matrix is diagonal insofar as the reactants and products are concerned, so that we may write

$$\rho DY_i/Dt - \underset{\sim}{\nabla}\cdot(\mu_{ii}\underset{\sim}{\nabla}Y_i) = \dot{\rho}_i \quad \text{for} \quad i = 1,2,\ldots,N\text{-}1. \tag{6}$$

Here $\dot{\rho}_i$ is the mass production rate per unit volume of the ith component; its precise form is considered below. The equation for the mass fraction Y_N of the inert is more complicated; but it can be obtained from the relation

$$\sum_{i=1}^{N} Y_i = 1 \tag{7}$$

instead, once the other Y_i's have been determined.

Coupling between the fluid-mechanical equations (1), (2) and the thermal-chemical equations (4),(6) occurs because of density variations. If these variations are ignored, the former may be solved for $\underset{\sim}{v}$, which can then be substituted into the latter, a substantial simplication.

Such a procedure is justified if the heat released by the reaction is small, but this is not a characteristic of combustion systems, whose main purpose is to liberate heat from its chemical bonds. For this reason, the simplified system of equations should be thought of as a model in the spirit of Oseen's approximation in hydrodynamics. However, to emphasize the mathematically rational nature of the procedure, we shall refer to the simplified system as the constant-density approximation rather than model. Phenomena whose physical basis is truly fluid-mechanical (e.g. the Darrieus-Landau instability discussed in lecture 5) are not encompassed by this approximation, but much of importance is; it will play a central role in our discussion.

There remains the question of the contribution of the individual reactions to the heat release q and the production rates $\dot{\rho}_i$. It is possible, in principle, to consider all the reactions that are taking place between the constituents of a mixture. However, this is done but infrequently; often a complete chemical-kinetic description (i.e. how the rates depend on the various concentrations and temperature, or even whether a particular reaction takes place) is not available. Even when it is, its complexity may deter solution by anything short of massive use of computers. For these reasons, simplified kinetic schemes are normally adopted which model, in an overall fashion, the multitude of reactions.

The simplest are the one-step irreversible schemes that account for the consumption of the reactants, here taken to be just a fuel and an oxidant. If the reactants are simply lumped together as a single entity, the scheme is represented by

$$[Y_1] \rightarrow \text{products}, \qquad (8)$$

where brackets denote a molecule of the component whose mass fraction is enclosed. On the other hand, if the separate identities of the fuel and oxidant are recognized, we have

$$\nu_1[Y_1] + \nu_2[Y_2] \rightarrow \text{products}; \qquad (9)$$

here the ν_i are stoichiometric coefficients, specifying the molecular proportions in which the two reactants participate. We shall adopt the scheme (8) when discussing premixed combustion and (9) for *diffusion flames* (lectures 8-10 only). These terms are defined at the beginning of section 4.

If N_i is the number density of the i^{th} component, so that

$$\dot{\rho}_i = m_i \dot{N}_i, \qquad (10)$$

where m_i is the molecular mass of the ith component, the reaction rate ω is defined by the formula

$$\dot{N}_i = -\nu_i \omega. \qquad (11)$$

It is then common to write

$$\omega = k(T)\rho^\gamma \prod_j Y_j^{\beta_j} \quad (\gamma, \beta_j \text{ positive consts.}) \qquad (12)$$

for the reaction rate, an empirical formula that is suggested by a theoretical treatment of so-called elementary reactions. The product contains a single term for the scheme (8), two terms for (9). The Arrhenius law

$$k = BT^\alpha e^{-E/RT} \quad (B, \alpha, E \text{ consts.}), \qquad (13)$$

which we shall adopt, is at the heart of our mathematical treatment; E is called the activation energy.

The heat release q is a consequence of the difference between the heats of formation of the products and those of the reactnats, so that it is proportional to ω. Combustion is inherently *exothermic*, so that we shall write

$$q = Q\omega, \qquad (14)$$

where Q(>0) has the dimensions of energy.

2. Nondimensional Equations and Their Shvab-Zeldovich Formulation.

We shall take units as follows:

$$\text{temperature } Q/c_p \sum_j \nu_j m_j \text{ (summation over 1 or 2 reactants)} \qquad (15)$$

$$\text{pressure } p_c\text{, density } \rho_r\text{, mass flux } M_r\text{, speed } M_r/\rho_r, \qquad (16)$$

$$\text{length } \lambda/c_p M_r, \quad \text{time } \lambda\rho_r/c_p M_r^2\text{, pressure variations } M_r^2/\rho_r. \qquad (17)$$

Appropriate choices for the reference density ρ_r and the reference mass flux M_r will be made according to the problem considered. The governing equations in nondimensional form are

$$\rho T = m p_c c_p \sum_j \nu_j m_j/\rho_r RQ, \quad \partial\rho/\partial t + \underset{\sim}{\nabla}\cdot(\rho \underset{\sim}{v}) = 0, \qquad (18)$$

$$\rho D\underset{\sim}{v}/Dt = -\underset{\sim}{\nabla}p + \mathcal{P}[\nabla^2\underset{\sim}{v} + \tfrac{1}{3}\underset{\sim}{\nabla}(\underset{\sim}{\nabla}\cdot\underset{\sim}{v})], \qquad (19)$$

$$\rho DT/Dt - \nabla^2 T = \Omega, \quad \rho DY_i/Dt - \mathcal{L}_i^{-1}\nabla^2 Y_i = \alpha_i\Omega, \qquad (20)$$

where i runs from 1 to N-1, and

$$\mathcal{P} = \kappa c_p/\lambda \text{ (Prandtl number)}, \quad \mathcal{L}_i = \lambda/\mu_{ii}c_p \text{ (Lewis number)}, \qquad (21)$$

$$\alpha_i = -\nu_i m_i/\sum_j \nu_j m_j \text{ (with } \sum_i \alpha_i = -1\text{)}, \quad \Omega = \mathcal{D}e^{-\theta/T}\prod_j Y_j^{\beta_j}, \qquad (22)$$

$$\theta = Ec_p \sum_j \nu_j m_j/QR, \quad \mathcal{D} = DM_r^{-2}, \quad D = [\lambda B Q^\alpha \rho_r^\gamma/c_p^{1+\alpha}(\sum_j \nu_j m_j)^{\alpha-1}]\rho^\gamma T^\alpha. \qquad (23)$$

Except in the case $\gamma = \alpha$, the so-called Damköhler number $\mathcal{D}$ is variable; it is called a number in spite of having the dimensions of M_r^2. In the context of activation-energy asymptotics ($\theta \to \infty$), only its value at a fixed temperature T_* plays a role, so that it may be considered an assigned constant.

When one of the Lewis number L_i is equal to 1, the differential operator in its equation (20b) is identical to that in equation (20a). We may therefore write

$$(\rho D/Dt - \nabla^2)(T - Y_i/\alpha_i) = 0, \qquad (24)$$

of which one solution is

$$T - Y_i/\alpha_i \equiv H_i \qquad 25)$$

constant. If this solution is appropriate for the problem at hand, Y_i may be eliminated in favor of T, thereby reducing the number of unknowns. The linear combusion (25) is known as a Shvab-Zeldovich variable; it is easier to find by virtue of satisfying the reactionless equation (24).

3. Activation-Energy Asymptotics

In these lectures we shall discuss a variety of combustion phenomena on the basis of equations (18)-(20). To do this we need an effective tool for dealing with the highly nonlinear reaction term Ω. Activation-energy asymptotics, used in an ad hoc fashion by the Russian school (notably Frank-Kamenetskii and Zeldovich) in the 40's, exploited in the framework of modern singular perturbation theory (but in a very narrow context) by aerothermodynamicists in the 60's, and systematically developed by Western combusion scientists in the 70's, is just such a tool.

The limit $\theta \rightarrow \infty$ is, by itself, of little interest: the definition (22b) shows that Ω vanishes. To preserve the reaction, it is necessary for $\mathcal{D}$ to become unboundedly large, i.e. we must consider a distinguished limit characterized essentially by

$$\mathcal{D} \sim e^{\theta/T_*} \qquad (26)$$

where T_* is a constant that may have to be found. The consequences of this limit then depend on the relative magnitudes of T and T_*.

For $T < T_*$, the reaction term Ω vanishes to all orders; this is known as the frozen limit. For $T > T_*$, equations (20) imply $\prod_j Y_j^{\beta_j} \to 0$ exponentially rapidly, so that at least one Y_i vanishes like that, and again Ω vanishes to all orders; the equilibrium limit holds. For T no more than $O(\theta^{-1})$ from T_*, reaction takes place, usually in a thin layer called a flame sheet. Thus, with a few exceptions, the general feature of high activation energy is the absence of chemical reaction from most of the combustion field, the description of which is thereby simplified. Reaction occurs only in thin layers (spatial or temporal), whose description is also relatively simple.

4. Plane Deflagration Waves.

We are now ready to demonstrate the efficacy of the technique that is the central theme of these lectures, by examining the fundamental problem of premixed combustion - the plane unbounded flame. But first we pause for a few words on terminology.

In general, two-reactant flames can be classified as diffusion or premixed. In a premixed flame the reactants are mixed and burn when the mixture is raised to a sufficiently high temperature. In a diffusion flame the reactants are of separate origin; burning occurs only at a diffusion-blurred interface.

Both kinds of flames can be produced by a Bunsen burner (figure 1). If the air hole is only partly open, so that a fuel-rich mixture of gas and air passes up the burner tube, a thin conical sheet of flame stands at the mouth; this is the premixed flame. Any excess gas escaping downstream mixes by diffusion with the surrounding atmosphere and burns as a diffusion flame.

Separate origins do not guarantee a diffusion flame, however. In figure 2 the reactants are originally separated by the splitter plate but mix before igniting. The flame spread across the oncoming flow is therefore premixed. Behind this premixed flame the remaining portions of the reactants are separate again, so that a diffusion flame trails downstream.

The plane unbounded flame of premixed combustion, the so-called (plane) deflagration wave, propagates at a well-defined speed through the fresh mixture and, accordingly can be brought to rest by means of a counterflow. It is natural to take the mass flux of this counterflow as the representative mass flux M_r; the counterflow is not known a priori, but is to be determined during the analysis of the combustion field. Indeed, its determination is the main goal of the analysis. A choice must also be made of the reference density ρ_r; we shall take it to be that of the fresh mixture.

The continuity equation (18b) integrates to give

$$\rho v = 1, \tag{27}$$

so that

$$dT/dx - d^2T/dx^2 = \Omega. \tag{28}$$

Since there is only one reactant we shall drop the subscript 1. For $L = 1$ in the corresponding equation (20b), the Shvab-Zeldovich formulation applies, showing that

$$T+Y \equiv H = T_f+Y_f \equiv T_b, \tag{29}$$

where the subscript f denotes the fresh mixture at $x = -\infty$. (Actually, H is the total enthalpy of the mixture). Thus,

$$\Omega = \mathcal{D}(T_b - T)e^{-\theta/T} \tag{30}$$

if the most common choice $\beta_1 = 1$ is made. Equations (28) and (30) form a single equation for T, which must satisfy the boundary condition

$$T \to T_f \quad \text{as} \quad x \to -\infty. \tag{31}$$

The requirement that all the reactant be burnt provides the final boundary condition

$$T \to T_b \quad \text{as} \quad x \to +\infty. \tag{32}$$

Note that neither the equation of state (18a) nor the momentum equation (19) has been used; the former provides ρ once T has been found, and the latter then determines p from $v = 1/\rho$.

It is immediately apparent, since Ω does not vanish for $T = T_f$, that the problem for T cannot have a solution. The mixture at any finite location will have an infinite time to react and so will be completely burnt. This cold-boundary difficulty, as it is known, is a result of idealizations and can be resolved in a number of ways: the mixture can originate at a finite point; an appropriate initial-value problem can be defined, without the solution having a steady limit of the kind originally sought; or a switch-on temperature can be introduced below which Ω vanishes identically. It is one of the virtues of activation-energy asymptotics that it makes such resolutions unnecessary. Reaction at all temperatures below T_* (including T_f) is exponentially small, so that it takes an exponentially large time for it to have a significant effect; in other words, T_* is a switch-on temperature. Consequently, it is not necessary to discuss the cold-boundary difficulty any further.

We now seek a solution that is valid as $\theta \to \infty$. Our construction will be guided by the assumption that, in the limit, reaction is confined to a thin sheet located at $x = 0$. On either side of this flame sheet, equation (28) simplifies to

$$dT/dx - d^2T/dx^2 = 0, \tag{33}$$

which only has a constant as an acceptable solution behind the flame sheet ($x > 0$), exponential growth being excluded. The boundary condition (32) then shows that

$$T = T_b \quad \text{for} \quad x > 0; \tag{34}$$

T_b is called the adiabatic flame temperature. It follows that the temperature at the flame sheet is T_b, so that this is also the value of T_* needed to specify the distinguished limit (26).

Ahead of the flame sheet, equation (33) has the solution

$$T = T_f + Y_f e^x \text{ for } x < 0, \tag{35}$$

satisfying the boundary condition (31) and making T continuous at $x = 0$. No structure could be found for the flame sheet if the temperature were discontinuous.

Turning now to the structure, which must determine the still unknown M_r (i.e. $\mathcal{D}$), we note that the form of Ω restricts the variations in T to being $O(\theta^{-1})$. Since the temperature gradient must be $O(1)$ to effect the transition between the profiles (34) and (35), the appropriate layer variable is

$$\xi = \theta x; \tag{36}$$

coefficients in the layer expansion

$$T = T_b - \theta^{-1}T_b^2\phi + \dots \text{ with } \phi = (1/T)_1 \tag{37}$$

are now considered to be functions of ξ. Equation (28) then shows that

$$d^2\phi/d\xi^2 = \tilde{\mathcal{D}}\phi e^{-\phi} \text{ with } \tilde{\mathcal{D}} = \mathcal{D}e^{-\theta/T_b}/\theta^2, \qquad (38)$$

while matching with the solutions (34), (35) gives the boundary conditions

$$\phi = -Y_f\xi/T_b^2 + o(1) \text{ as } \xi \to -\infty, \quad \phi = o(1) \text{ as } \xi \to +\infty. \qquad (39)$$

In order for this problem (in ϕ) to make sense, $\tilde{\mathcal{D}}$ must be $O(1)$. Then $\mathcal{D}e^{-\theta/T}$ is $O(\theta^2)$ in $x > 0$, so that equation (28) is unbalanced unless $Y = 0$ (to all orders) behind the flame sheet, consistent with the result (34). Thus, equilibrium prevails in $x > 0$ even though the mixture is no hotter than the flame sheet there.

Integrating equation (38a) once, using the condition (39b), gives

$$(d\phi/d\xi)^2 = 2\tilde{\mathcal{D}}[1-(\phi+1)e^{-\phi}]. \qquad (40)$$

The remaining boundary condition will then be satisfied only if

$$\tilde{\mathcal{D}} = Y_f^2/2T_b^4, \qquad (41)$$

corresponding to the determination

$$M_r = \sqrt{2D}\, T_b^2\, e^{-\theta/2T_b}/Y_f\theta \qquad (42)$$

of the burning rate. (If D is temperature dependent it must be evaluated at the temperature T_b.)

Determination of the wave speed M_r/ρ_r is the main goal of the analysis, and rightly so. But, at the same time, the structure of the combustion field is obtained (figure 3). The reaction zone appears as a discontinuity in the first derivatives of T and Y, a reflection of the delta function nature of Ω in the limit $\theta \to \infty$. Ahead, the temperature rises and the reactant concentration falls as the reaction zone is approached through the so-called preheat zone. It is the preheat zone that delimits the combustion field and, therefore, defines the thickness of the flame. According to the formula (35), more than 99% of the increase in temperature from T_f to T_b is achieved in a distance 5, i.e. $5\lambda/c_p M$ in dimensional terms. With this definition of flame thickness, we find that hydrocarbon-air flames are about 0.5 mm thick. The thickness of the reaction zone, which is scaled by θ^{-1}, is typically 10 or 20 times smaller.

5. Generalizations.

If the reaction-zone structure itself is required, equation (40) must be integrated to obtain ϕ as a function of ξ. The constant of integration is fixed by the boundary condition (39a), which is thereby used a second time. The three requirements that the boundary conditions impose on the solution of the second-order equation (38a) are responsible for a definite value of $\mathcal{D}$. The term laminar-flame eigenvalue is often used.

The analysis in section 4 was carried through with Lewis number unity for the sake of simplicity alone. For $\mathcal{L} \neq 1$, the formula (42) is replaced by

$$M_r = \sqrt{2\mathcal{L}D}\, T_b^2\, e^{-\theta/2T_b}/Y_f\theta, \tag{43}$$

The only change is the replacement of $\sqrt{2D}$ by $\sqrt{2\mathcal{L}D}$.

The rate at which the mixture burns is extremely sensitive to the flame temperature. If T_b changes to $T_b - \theta^{-1}T_b^2\phi_*$, i.e. by an $O(\theta^{-1})$ amount, the burning rate changes to

$$M = M_r e^{-\phi_*/2}, \tag{44}$$

i.e. by an O(1) amount. This result has general validity, i.e. it holds whatever the nature of the perturbation, steady or unsteady. The reason is that, in determining the eigenvalue $\mathcal{D}$, the perturbation only intrudes through the matching of ϕ at $\xi = +\infty$ (which leads to the exponential factor); matching ahead of the flame sheet is with an $O(1)$ gradient that is unaffected by the perturbation.

Questions involving deflagration waves are essentially free-boundary problems: the location of the flame sheet and the combustion fields on either side have to be determined simultaneously. In that context, the structure problem (38), (39), modified for $O(\theta^{-1})$ perturbations in flame temperature, provides a leading-order jump condition on the normal derivative $\partial T/\partial n$, namely

$$\delta[(\partial T/\partial n)^2] = Y_f^2\, e^{-\phi_*} \tag{45}$$

when M_r is taken to have the value (42). This, the true role of the structure problem, is obscured by the analysis of the steady plane wave given in the last section, where M_r was taken to be the constant (unknown) burning rate. If M_r had been given the value (42) without explanation, and M used to denote the (dimensionless) burning rate, then x would have been replaced by Mx in the formula (35) and the jump condition (45) would have yielded

$$M = 1, \tag{46}$$

i.e. the location of the flame sheet.

When the temperature gradient vanishes to leading order behind the flame sheet, the jump condition (45) gives the gradient

$$\partial T/\partial n = Y_f e^{-\phi_*/2} \tag{47}$$

ahead. This result will be needed repeatedly later.

In many circumstances, locating the flame sheet is relatively easy. In the final lecture we shall discuss several problems in which it is the principal question.

REFERENCE

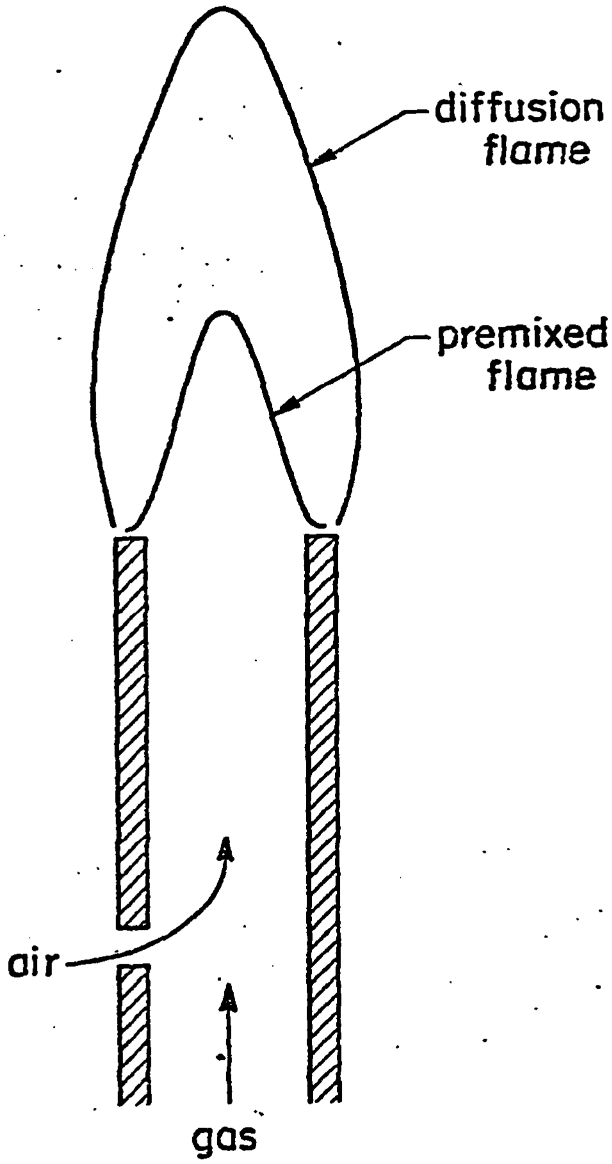
1. Buckmaster, J. & Ludford, G.S.S. (1982). Theory of Laminar Flames. Cambridge: University Press.

Figure Captions

2.1 Bunsen burner.

2.2 Combustion of initially separated reactants.

2.3 Profiles of T and Y, drawn for $L = 1$ and $T_f = 0.25$, $Y_f = 0.75$.



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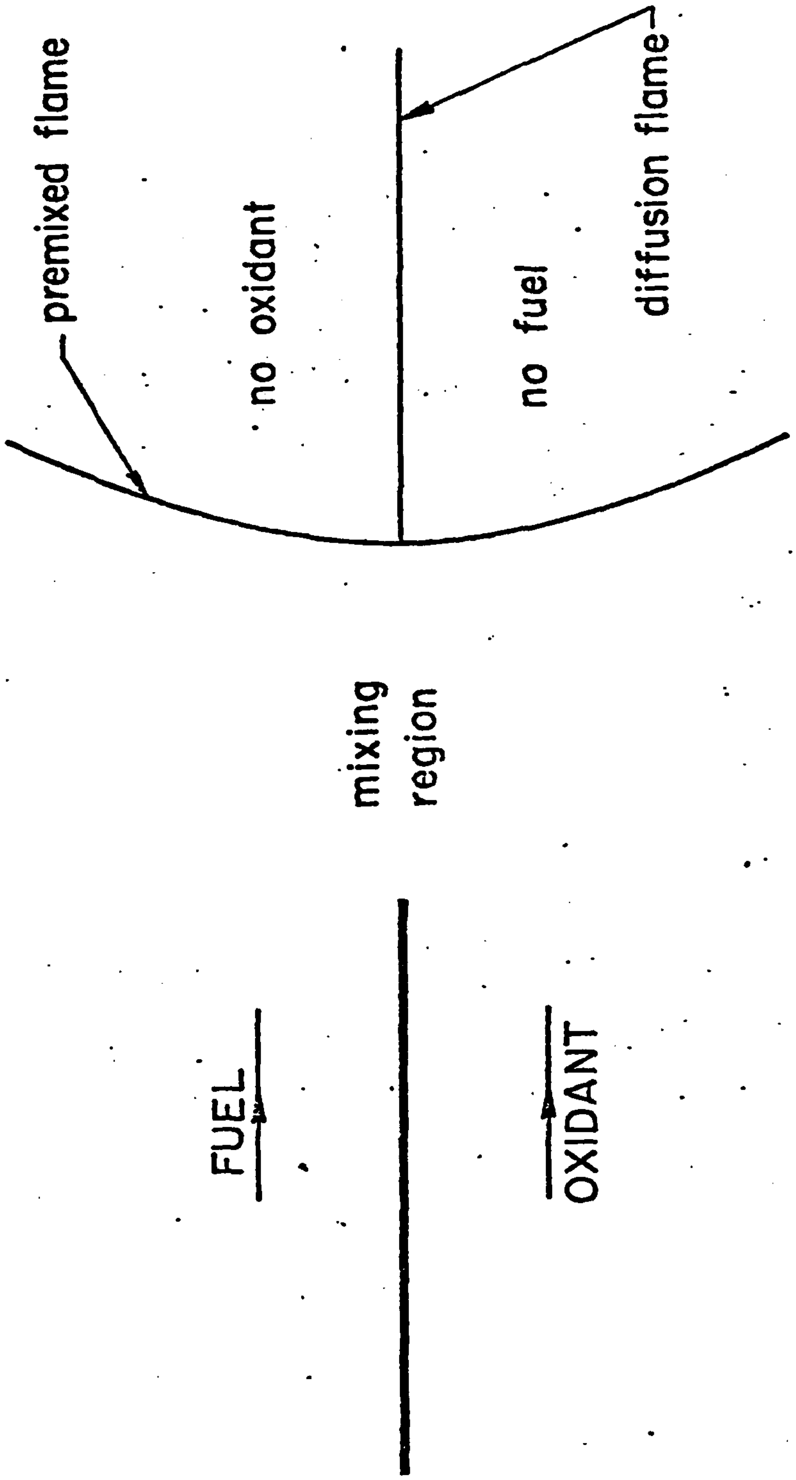
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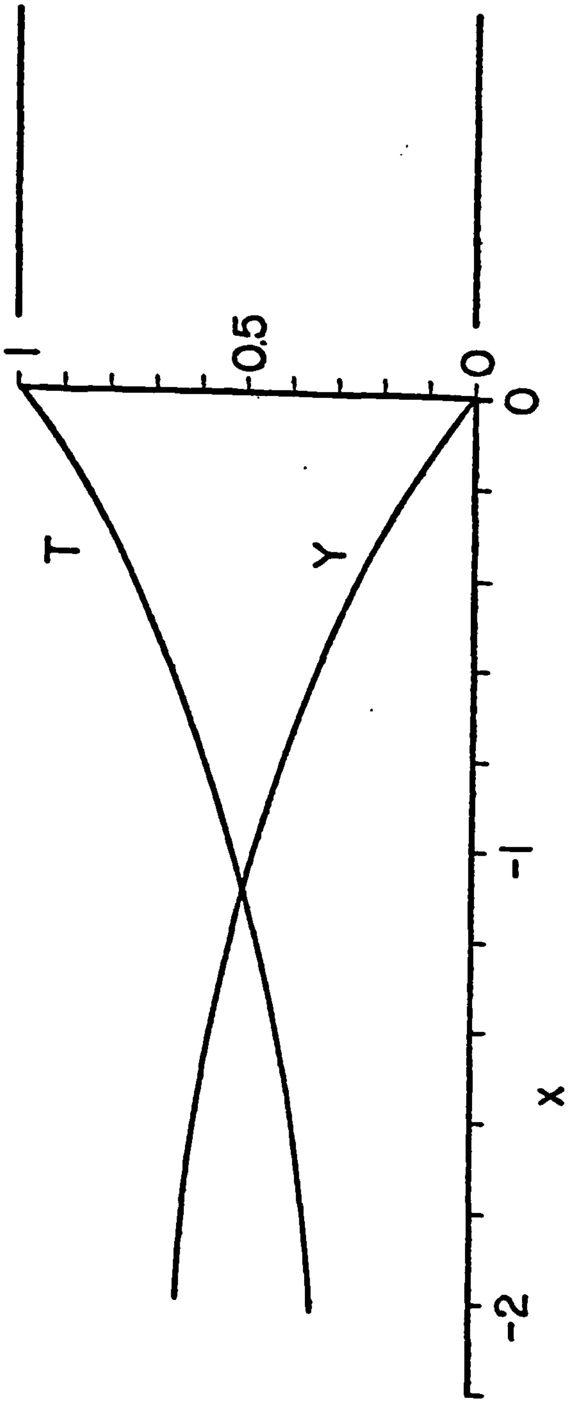
no oxidant
no fuel
diffusion flame
mixing region
FUEL
OXIDANT

2.2

2.3



REPORT DOCUMENTATION PAGE		**READ INSTRUCTIONS BEFORE COMPLETING FORM**
1. REPORT NUMBER 147	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) LECTURES ON MATHEMATICAL COMBUSTION Lecture 2: Governing Equations, Asymptotics, and Deflagration		5. TYPE OF REPORT & PERIOD COVERED Interim Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) J.D. Buckmaster and G.S.S. Ludford		8. CONTRACT OR GRANT NUMBER(s) DAAG29-81-K-0127
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Theoretical and Applied Mechanics Cornell University, Ithaca, New York 14853		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS P-18243-M
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709		12. REPORT DATE January 1983
		13. NUMBER OF PAGES 19
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release: distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Dilute mixture, constant-density approximation, Arrhenius law, Shavg-Zeldovich formulation, Damkohler number, Lewis number, activation-energy asymptotics, frozen and equilibrium limits, deflagration wave, diffusion and premixed flames, cold-boundary difficulty.

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

The problem of formulating the governing equations of combusion consists, at its simplest, in characterizing the flow of a viscous, heat-conducting mixture of diffusing, reacting gases. This is a formidable task that could fill a week of lectures by itself, most of which would not be of great interest to a mathematical audience. Mindful of this, we shall limit ourselves to a description, rather than a derivation, of the simplest equations that can be brought to bear on combustion problems. Only the most important assumptions

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