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MATHEMATICAL THEORY OF LAMINAR COMBUSTION XII.

Ignition and Explosion.

Technical Report No. 114

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March 1980

Technical repts.

TR-114

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

Contract No. DAAG29-79-C-0121

15882.16-M

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Foreward

This report is Chapter XII of the twelve in a forthcoming research monograph on the mathematical theory of laminar combustion. Chapters I-IV originally appeared as Technical Reports Nos. 77, 80, 82 & 85; these were later extensively revised and then issued as Technical Summary Reports No's 1803, 1818, 1819 & 1888 of the Mathematics Research Center, University of Wisconsin-Madison. References to I-IV mean the MRC reports.

Contents

Chapter XII

Ignition & Explosion

1. Synopsis.

The phenomenon of ignition has already been encountered in at least three contexts: burning of a linear condensate (Ch. IV), spherical diffusion flame (Ch. VI) and spherical premixed flame (Ch. VII). From the S-shaped response curves determined by steady-state analyses it was argued that the burning rate would jump from a weak, almost extinguished, level to a vigorous one as the pressure (and hence the Damköhler number) is increased through some critical value (corresponding to the lower bend of S). An intrinsically unsteady phenomenon, appropriately called ignition in these contexts, was thereby inferred from existence results for the steady state.

Such analyses have a fairly long history in combustion, the simplest example being the thermal theory of spontaneous combustion identified with the name of its originator, Frank-Kamenetskii (1969). Sec. 2 will give a mathematical version of that theory, which shows an early appreciation of activation-energy asymptotics (though not in the formal sense of the present monograph).

Useful though steady-state analyses undoubtedly are, such phenomena demand unsteady descriptions; and that is the main goal of the present chapter. The three contexts already encountered are, however, too complicated for our purposes and we turn instead to a simpler problem containing the essential feature, namely the evolution of a deflagration wave from an unburnt state.

Consider a thermally insulted enclosure containing a mixture at
sufficiently low temperature for the reaction though present, to be very
weak. Since the heat released cannot escape the temperature must rise,
albeit very slowly. After a long time the heat generated by the initially
weak reaction will have raised the temperature of the mixture enough to
excite rapid reaction somewhere and, if the combustion field is inhomogeneous,
a deflagration wave will sweep across it. To distinguish this type of
rapid reaction from that caused by external agencies, the term thermal
explosion is used. (Thermal refers to the temperature sensitivity of the
reaction rate. Another type of explosion is due to a rapid chain reaction
being initiated when conditions are such that a few necessary radicals are
produced from one of the reactants.)

A spatially homogeneous explosion is described by ordinary differential
equations. Its study in Sec. 3 provides insight into the mathematical nature
of the rapid transients characteristic of the explosion process. That
prepares the way for a discussion of the spatially inhomogeneous problem
in Sec. 4.

A distinctive feature of thermal explosion is the very rapid temperature
increase, known as thermal runaway, that occurs at the end of a well-defined
induction period. The mathematical manifestation is unboundedness in the
solution of an equation for small perturbations of the initial state.
(Evolution equations that generate unboundedness solutions after a finite
time have recently attracted the attention of mathematical analysts.) The
subject of the thermal ignition provides other examples, one of the simplest
being a half space filled with a combustible mixture, at the boundary of
which a positive heat flux is applied. After a certain time, ignition

occurs at the boundary and a plane deflagration wave propagates into the interior, consuming the mixture in its passage. The early stages of the process are described in Sec. 5.

The problems in Secs. 2-5 are all concerned with reactants that are premixed; a whole range of such problems, to which activation-energy asymptotics could be profitably applied, is discussed by Merzhanov & Averson (1971). By contrast Sec. 6 treats the so-called Marble-Adamson (1954) problem, in which a fuel and oxidant in separate half-spaces are brought into contact at the initial instant so as to interdiffuse and burn. There are many points of similarity with the spatially inhomogeneous thermal explosion, and a reasonably complete description of the combustion process is possible.

2. Spontaneous Combustion.

Exothermic chemical-reaction is a well-known hazard of certain bulk materials in storage or transit. Joseph Conrad in his story "Youth" graphically describes the peril. Take one ship with a cargo of coal dampened down because of an earlier leak (now fixed); embark on a slow voyage to Bangkok; and before the China Sea is reached the legend "Do or Die" proves ominous rather than brave.

Any moist volume of organic material (e.g. wood chips, wool, corn cobs, compost) will, because of chemical reaction initiated by micro-organisms, get hot. (The reduction of spontaneous reactions in fruits and vegetables is a major concern of post-harvest physiologists.) Certain inorganic material such as ammonium nitrate, lead azide or a hydrogen sulphide/oxygen mixture will also heat up because of chemical decomposition.

If the reaction were independent of temperature there would be a maximum, depending on the dimensions, to which the temperature of a volume of material would rise after a long time. (That maximum holds steady over an even longer period, but there is an eventual decay due to reactant depletion.) In the quasi-steady state the rate of generation of heat, which is proportional to a^3 for a volume of characteristic dimension a, would be balanced by loss through the surface, which is proportional to a^2 with a factor of proportionality an increasing function of temperature there. Clearly the larger the volume in equilibrium the hotter it would be. However, the reaction does depend on temperature, proceeding much more vigorously at higher temperatures, so that there will be a critical value of a beyond which the efflux at the surface is insufficient to dispose of the heat generated and unsteady combustion will occur. Our first task then is to look for steady states.

Any steady state is described in equation (I.56) with $\partial/\partial t = v = 0$, i.e.

(1) $$\nabla^2 T = -\Omega \quad \text{where } \Omega = De^{-\theta/T},$$

the latter being appropriate when the length a is used in non-dimensionalization. For solids, the density has a constant value, which may be designated ρ_c so as to replace ρ by 1 in the definition (I.59) of D; pressure does not arise, which means that $\overline{p}_c$ should be replaced by $\rho_c QR/c_p m$ in that definition (thus eliminating the gas constant R from it); and α is usually taken to be zero. The only new assumption is that reactant depletion may be neglected (the constant mass fractions in Ω being absorbed into D) because the steady state is close to the initial state, a condition ensured a posteriori when θ is large. For gases, of primary interest to us,

there is the additional assumption of small heat release so that the constant
density approximation can be made to ensure that the mixture stays effectively
at rest.

For an initially uniform temperature T_0 such as we have so far
envisaged, this purely thermal problem can be treated in the limit $\theta \to \infty$
by setting

(2)
$$T = T_0 + \theta^{-1}T_1 + o(\theta^{-1}).$$

To ~~next~~ *first* order we find

(3)
$$\nabla^2 \phi = -\delta e^\phi,$$

where

(4)
$$\phi = T_1/T_0^2 \quad \text{and} \quad \delta = D\theta e^{-\theta/T_0}/T_0^2.$$

Note that the steady state being sought is close to the initial state,
so that neglect of reactant depletion is justified. However, for natural
organic materials such as wood chips the activation energy is not large
and depletion is not small; in either circumstance the present analysis
is not appropriate.

The approximation (2) is familiar from our earlier ignition studies
(Secs. VI.4 & VII.6). In the present context it is due to Frank-Kamenetskii,
constituting an early example of activation-energy asymptotics. References
and a discussion of the solutions of equation (3) are given in his book
(1969). On the other hand, linearization of the exponent θ/T in the
Arrhenius factor has sometimes been adopted as a model not rationally
consistent (in an asymptotic sense) with the underlying equation (1) for

the specific problem being examined. The plane form of equation (3) has a long history (Stuart (1967), going back at least to Liouville (1853), to whom it is sometimes attributed. The general solution is known, but there appears to be no way of fitting it to boundary conditions of interest. As a consequence, solutions of complete boundary-value problems have only been constructed in a few special cases.

Amongst these are problems depending on x alone. Indeed the corresponding problems for the exact equation (1) can then be solved, providing useful checks for the present asymptotics [cf. Shouman & Donaldson (1975)]. A particularly simple example is an infinite slab $|x| \leq 1$ of combustible material whose surfaces are held at the temperature T_0, so that

$$(5) \qquad \phi = 0 \quad \text{for} \quad x = \pm 1.$$

Such a surface condition corresponds to the limit of an efflux $k(T - T_0)$ per unit area as $k \to \infty$, and it is the ility of the material in the slab to conduct that heat to the surfaces which determines whether a steady state exists or not. By symmetry ϕ will attain its maximum, ϕ_m say, at $x = 0$; and in terms of it we have

$$(6) \qquad \phi = 2 \, \ell n \, [e^{\phi_m/2} \, \text{sech}(\sqrt{\tfrac{1}{6}e^{\phi_m}/2} \, x)].$$

(Cf. Fig. 2a for a graph of this function.) The boundary conditions (5) therefore require

$$(7) \qquad \sqrt{\delta/2} = e^{-\phi_m/2} \, \cosh^{-1}\!\left(e^{\phi_m/2}\right),$$

a relation fixing the maximum temperature in terms of δ. For a given material δ can be varied through a, the semi-thickness of the slab,

or T_0, the temperature at its surfaces [see equation (4b) and the definition (I.60) of D].

Fig. 1 shows the response (7), which has the typical shape of an ignition curve. There is a critical value

(8) $$\delta_c = .878.$$

above which no solution exists and below which there are two solutions. A value of δ greater than δ_c is said to be supercritical while a smaller value is said to be subcritical. The implication is that thick hot slabs, being supercritical, will burst into flames but thin cold slabs, being subcritical, will not; and this general picture has been confirmed experimentally for a number of substances.

The symmetry of the boundary conditions makes the solution atypical however, as we shall see from another example in which the surfaces $x = \pm 1$ are held at temperatures T_0 and αT_0, respectively, where $0 < \alpha < 1$. Now the reaction is confined to a neighborhood of the hot boundary in the limit $\theta \to \infty$ instead of being spread across the slab, so that conduction of its heat to that surface is much easier and δ_c is much larger.

The initial temperature in the slab, due entirely to conduction, is

(9) $$T = [1 + \alpha + (1 - \alpha)x]T_0/2$$

and we seek a steady state within $O(\theta^{-1})$. For such a state the $O(1)$ temperature has its maximum at the hot boundary, so that reaction only occurs in a zone near there. The expansion (2) is still valid, but its variable is now

(10) $$\xi = \theta(1 - x).$$

The structure of the reaction zone is found to be governed by

$$(11) \qquad d^2\phi/d\xi^2 = -\tilde{\delta}e^\phi \quad \text{with } \tilde{\delta} = \theta^{-2}\delta$$

and

$$(12) \qquad d\phi/d\xi = (1-\alpha)/2T_0 + o(1) \text{ as } \xi \to -\infty, \phi = 0 \text{ for } \xi = 0,$$

where the first boundary condition comes from matching with the temperature (9) outside the zone. The general solution of equation (11) is

$$(13) \qquad \phi = 2 \ln \left\{ e^{\phi_0/2} \text{sech}[\sqrt{\tilde{\delta}e^{\phi_0}/2}(\xi - \xi_0)] \right\}$$

where ξ_0 is the location of the maximum ϕ_0; and to satisfy the conditions (12) we must set

$$(14) \qquad \tilde{\delta} = \frac{(1-\alpha)^2}{8T_0^2} e^{-\phi_0} \quad \text{and} \quad \xi_0 = \pm\left(\frac{2}{\tilde{\delta}e^{\phi_0}}\right)^{1/2} \text{sech}^{-1}(e^{-\phi_0/2}).$$

Since ϕ vanishes at the surface, ϕ_0 ranges from 0 to ∞ (otherwise ξ_0 is complex), so that δ cannot exceed

$$(15) \qquad \tilde{\delta}_c = (1-\alpha)^2/8T_0^2.$$

The ± signs on ξ_0 provide two solutions when $\tilde{\delta} < \tilde{\delta}_c$ (see Fig. 2a); for the plus sign, ξ_0 lies outside the slab and the maximum t. in the slab is zero (its surface value) and not ϕ_0. If ϕ_m denotes this maximum, then

$$(16) \qquad \phi_m = \begin{cases} \phi_0 & \text{for } \xi_0 < 0, \\ 0 & \text{for } \xi_0 > 0 \end{cases}$$

and the relation (14) leads to the response shown in Fig. 2b.

Note that $\tilde{\delta} = \theta^{-2}\delta$ implies that the D corresponding to $\tilde{\delta}_c$ is much larger than that corresponding to δ_c. We conclude that raising the temperature of the cold boundary to that of the hot will greatly increase the risk of explosion. In fact the formula (15) suggests that the risk increases sharply as soon as α is within $O(\theta^{-1})$ of 1.

Two further points should be noted. The second problem illustrates ignition rather than explosion. With an ambient temperature αT_0, an external agency is required to raise the surface temperature at $x = 1$ to T_0; and if that is ultimately done slowly enough the conduction profile (9) will be established. Also we note that nothing has been missed in either problem by looking for steady states within $O(\theta^{-1})$ of the initial state. Any steady state further away would correspond to a D of exponential order θ/T_m, where the maximum temperature T_m is greater than T_0. It would therefore correspond to the origin in Figs. 1 and 2b.

For a review of the subject, including other geometries and boundary conditions, see Gray & Lee (1967). They do not use formal asymptotics, and indeed there is room for a comprehensive treatment doing so.

3. Adiabatic Explosion.

To describe an unsteady phase of the combustion, equation (1) is replaced by

$$(17) \qquad \partial T/\partial t - \nabla^2 T = De^{-\theta/T}$$

so that the small-disturbance equation (3) becomes

$$(18) \qquad \partial \phi/\partial t - \nabla^2 \phi = \delta e^{\phi}.$$

Th· problem is completed by the initial condition

(19) $\phi = 0$ for $t = 0$

and suitable boundary conditions.

The non-existence of a steady-state solution for the slab with equally hot surfaces and supercritical δ implies that ϕ must increase without bound, i.e. that T goes further than $O(\theta^{-1})$ from T_0. Indeed this happens at a finite time, as we shall now show for the spatially homogeneous problem of a material thermally insulated at its boundary surface, when equation (17) reduces to

(20) $dT/dt = De^{-\theta/T}$.

Our object in the present section is to gain insight into thermal explosions generally by examining those that are spatially homogeneous.

The corresponding small-disturbance equation is

(21) $d\phi/dt = \delta e^{\phi}$,

which has the solution

(22) $\phi = -\ell n(1 - \tau)$

satisfying the initial condition (19); here

(23) $\tau = \delta t$.

At the finite induction time δ^{-1}, the perturbation ϕ becomes unbounded and we speak of thermal runaway. Note that the phenomenon occurs for all values of δ in the spatially homogeneous problem because the heat generated

by the reactant cannot escape, i.e. conditions are adiabatic. On the other hand, if an artificial heat-loss term is introduced then subcritical behavior can be restored, see Kassoy & Poland (1975).

Clarification of the runaway process requires a return to equation (20). However, beyond thermal runaway a purely thermal model is of little practical significance since it predicts an unbounded increase in T, whereas the rise ceases when the reactant is consumed. Under the assumption that a single (decomposing) reactant is involved, its depletion can be incorporated by reinstating the mass fraction in equation (20), i.e. writing

$$\text{(24)} \qquad dT/dt = D(Y/Y_0)e^{-\theta/T},$$

and adding

$$\text{(25)} \qquad dY/dt = -D(Y/Y_0)e^{-\theta/T},$$

where Y_0 is the initial fraction of reactant in the material. Clearly the Shvab-Zeldovich relation

$$\text{(26)} \qquad Y + T = Y_0 + T_0 = H_0 \text{ (say)}$$

holds. No change in our analysis of the induction phase (Sec. 2) is necessary because Y then stays within $O(\theta^{-1})$ of Y_0 and hence may be replaced by it in equation (24). We are therefore led to the problem

$$\text{(27)} \qquad dT/dt = (T_0^2 \delta/Y_0\theta)(H_0 - T)\exp(\theta/T_0 - \theta/T), \quad T = T_0 \text{ for } t = 0.$$

Clearly T is monotonically increasing but the factor $(H_0 - T)$, corresponding to reactant depletion, ensures that it does not go beyond H_0; in fact it rapidly approaches H_0 (exponentially in time).

Kassoy (1975) has discussed the asymptotics of this problem directly; here we shall verify the salient features of his results from the exact solution. With the confidence so gained we shall attack spatially inhomogeneous problems in Sec. 4, for which there are no exact solutions against which to check the asymptotics. The exact solution here is expressed in terms of the exponential-integral function

$$(28) \qquad Ei(x) = \int_{-\infty}^{x} e^u \frac{du}{u},$$

where the principal-value sign is unnecessary for $x < 0$. With the time variable (23) we find

$$(29) \qquad T_0^2 \, e^{\theta/T_0}(\tau_e - \tau)/Y_0\theta = e^{\theta/H_0} \, Ei(\theta/T - \theta/H_0) - Ei(\theta/T),$$

where

$$(30) \qquad \tau_e = (Y_0\theta e^{-\theta/T_0}/T_0^2)[e^{\theta/H_0} Ei(\theta/T_0 - \theta/H_0) - Ei(\theta/T_0)].$$

Since

$$(31) \qquad Ei(x) = \ln|x| + O(1) \text{ as } x \to 0$$

the formula confirms that T approaches H_0 exponentially as
$\theta^{-1}\exp(\theta/T_0 - \theta/H_0)$ $\tau \to \infty$.

Three phases can be distinguished when θ is large: induction, explosion and relaxation. If T is bounded away from H_0, the arguments of both Ei-functions in the solution (29) become large so that, since

$$(32) \qquad Ei(x) = x^{-1}e^x[1 + x^{-1} + O(x^{-2})] \text{ as } x \to +\infty,$$

we find

(33) $\qquad \tau_e - \tau = [Y_0 T^2/T_0^2(H_0-T)]\exp(\theta/T - \theta/T_0)[1+O(\theta^{-1})],$

which reveals two of the phases. In the first phase T is still within $O(\theta^{-1})$ of T_0 and the right-hand side is $O(1)$, corresponding to induction. In fact, the result (22) is recovered when

(34) $\qquad \tau_e = 1 + T_0(2 + T_0/Y_0)\theta^{-1} + O(\theta^{-2})$

is noted. In the second phase T is bounded away from T_0 (as well as from H_0) and the right-hand side is exponentially small, showing that most of the change in T occurs within an exponentially small interval just before the time τ_e. In that sense τ_e is the time at which the explosion takes place.

The third, relaxation phase corresponds to values of T within $O(\theta^{-1})$ of H_0; then the argument of the first Ei-function in the solution (29) is $O(1)$ and we have

(35) $\qquad \tau_e - \tau = (Y_0\theta/T_0^2)\exp(\theta/H_0 - \theta/T_0)\mathrm{Ei}(\theta/T - \theta/H_0)[1 + O(\theta^{-1})].$

The final consumption of the reactnat also takes place within an exponentially small interval which, since the Ei-function changes sign at some positive values of its argument, spans τ_e.

We now turn to the question of deriving these asymptotic results directly from the governing equation (24). Consider first the induction phase and set

(36) $\qquad T = T_0 + \theta^{-1}T_1(t) + \theta^{-2}T_2(t) + O(\theta^{-3}).$

Then we find

$$(37) \qquad T_1 = -T_0^2 \ln(1 - \tau),$$

as in the earlier result (22), and

$$(38) \qquad T_2 = T_0^3 \left\{ \ln^2(1 - \tau) - (2 + T_0/Y_0)[\ln(1 - \tau) + \tau/(1 - \tau)] \right\}.$$

The logarithm in T_1 suggests that breakdown occurs when τ is exponentially close to 1, while the pole $(1 - \tau)^{-1}$ in T_2 changes that to algebraically close; and correctly so since the explosion time (34) is $O(\theta^{-1})$ away from 1. To restore exponential closeness it is only necessary to absorb the pole into T_1 by writing

$$(39) \qquad T_1 = -\ln[1 + T_0(2 + T_0/Y_0)\theta^{-1} - \tau],$$

which amounts to introducing the $O(\theta^{-1})$ approximation to τ_e. The same end can be achieved formally by considering both T and τ to be functions of a new time variable $\hat{\tau}$. If

$$(40) \qquad \tau = \hat{\tau} + \theta^{-1}\tau_1(\hat{\tau}) + O(\theta^{-2})$$

with

$$(41) \qquad \tau_1(0) = 0 \quad \text{and} \quad \tau_1(1) = T_0(2 + Y_0/T_0)$$

(τ_1 otherwise being arbitrary), then the explosion is fixed at $\hat{\tau} = 1$ and no pole occurs in $T_2(\hat{\tau})$. In short, the time to explosion has been determined asymptotically by considering only the induction phase; it is reasonable to suppose that the same procedure will work in other problems.

The description (33) of the explosion phase can also be derived directly from equation (24) but we shall not go into details. The most important

feature is the time scale

$$(42) \qquad \sigma = -\theta^{-1} \ln(\tau_e - \tau),$$

which plans a key role in the study of the inhomogeneous problem, as we shall see in Sec. 4. As σ ranges from 0 to $Y_0/T_0 H_0$ the temperature

$$(43) \qquad T = T_0/(1 - \sigma T_0) + O(1)$$

ranges from T_0 to H_0, to leading order.

For the final, relaxation phase we write

$$(44) \qquad T = H_0 + \theta^{-1} T_1(\omega) + o(\theta^{-2})$$

in equation (24), which shows that the appropriate time variable is

$$(45) \qquad \omega = (\tau - \tau_e)/\epsilon$$

where

$$(46) \qquad \epsilon = (Y_0 \theta/T_0^2) \exp(-\theta Y_0/H_0 T_0).$$

Then

$$(47) \qquad d\phi/d\omega = -\phi e^{\phi} \quad \text{with} \quad \phi = T_1 H_0^2,$$

the general solution of which is

$$(48) \qquad \omega - \omega_1 = Ei(1) - Ei(-\phi);$$

here ω_1 is just the value of ω when $\phi = -1$. The requirement that $\phi \to 0$ as $\omega \to +\infty$ (i.e. all reactant is consumed) is satisfied automatically, as is that of matching with the expansion (43). For the latter, note the

result

$$(49) \qquad \omega = e^{-\phi}/\phi$$

of introducing ω into the expansion (33) and then keeping it fixed under expansion. Comparison with the solution (48) shows that the integration constant ω_1 is left undetermined and in fact cannot be determined by asymptotic development: however many terms are retained in the expansion (33) it will never recapture the Ei-functions of the exact solution, whereas those functions determine ϕ. It is therefore fortunate that results analogous to

$$(50) \qquad \omega_1 = -Ei(1),$$

here obtained from the exact solution, will not be needed in the sequel.

4. Explosion with Heat Loss

Kassoy (1977) has incorporated non-adiabaticity into the spatially homogeneous problem by inserting a distributed heat-loss term proportional to $T - T_0$ into equation (24). Apart from the lack of a Shvab-Zeldovich relation, the new features are the inability of the reaction to produce the adiabatic temperature H_0 and the eventual decay to T_0. To obtain the essentially new phenomena of hot-spot formation and subsequent flash-through it is necessary to consider a more realistic problem involving spatial inhomogeneity, and that can be done without sacrificing the Shvab-Zeldovich relation.

Consider once more the infinite slab with equally hot surfaces. The equations (24,25) are now replaced by

$$(51) \qquad \partial T/\partial t - \partial^2 T/\partial x^2 = -(\partial Y/\partial t - \mathcal{L}^{-1}\partial^2 Y/\partial x^2) = D(Y/Y_0)e^{-\theta/T},$$

cf. equation (17). For a solid, where the reactant is unable to diffuse, the Lewis number $\mathcal{L}$ is infinite. Nevertheless we shall take $\mathcal{L} = 1$ so as to have the simplification of a Shvab-Zeldovich integral (26). Rather than maintaining the reactant there it would be more practical to prevent its flux. We shall see, however, that the boundary condition on Y does not influence the solution until after the main events have taken place. The problem we shall treat is therefore

$$(52) \qquad \partial T/\partial t - \partial^2 T/\partial x^2 = (T_0^2\delta/Y_0\theta)(H_0-T)\exp(\theta/T_0 - \theta/T)$$

$$(53) \qquad T = T_0 \quad \text{for} \quad t = 0 \quad \text{and for} \quad x = \pm 1.$$

By symmetry the condition at $x = -1$ can be replaced by

$$(54) \qquad \partial T/\partial x = 0 \quad \text{for} \quad x = 0,$$

with only the half-slab $0 \le x \le 1$ considered.

In addition to the induction, explosion and relaxation phases found in the spatially homogeneous problem (27) there are now transition and propagation phases. These arise because the explosion is here confined to a single location and then propagates elsewhere, involving a transition from the formation of a hot spot to the flash-through of a deflagration wave. These two new phases postpone the relaxation phase, which is the only feature affected by the boundary condition on Y.

As for the homogeneous problem, the induction phase is described by an expansion of the form (36), but now the coefficient functions depend on x also and $T_1 = T_0^2\phi$ satisfies

(55) $$\partial\phi/\partial t - \partial^2\phi/\partial x^2 = \delta e^\phi,$$

(56) $\partial\phi/\partial x = 0$ for $x = 0$, $\phi = 0$ for $x = 1$ and for $t = 0$.

If δ is greater than δ_c, as we shall suppose, the solution cannot tend to a steady limit. Since the solution of the corresponding homogeneous problem becomes unbounded in a finite time, it is not surprising to find that the same is true here (cf. Payne 1975 and Ayeni 1978). Thermal runaway can no longer occur everywhere when the surfaces are held at T_0 but is localized at the symmetry plane $x = 0$. The runaway time $\delta^{-1}\tau_e(\delta)$ is no longer fixed on the τ-scale, but is a function of δ that was first determined (numerically) by Poland (1979), see Kassoy & Poland (1980a), and then independently by Kapila (1980). As $\delta \downarrow \delta_c$ the time to runaway becomes indefinitely long.

While ϕ cannot be calculated analytically, its form as $\tau \to \tau_e$ can be determined, a step that is crucial for the subsequent development. Backward integration of a parabolic equation away from a singularity (in this case at $t = \delta^{-1}\tau_e$) is no novelty; more than thirty years ago Goldstein (1948) encountered such a question in his discussion of Prandtl's boundary-layer equations near a stagnation point. He showed that the similarity variable, here

(57) $$\eta = \delta^{1/2}x/(\tau_e - \tau)^{1/2},$$

plays a central role near the singularity. In terms of η,τ our equation becomes

(58) $$\partial\phi/\partial\tau - (\tau_e - \tau)^{-1}[\partial^2\phi/\partial\eta^2 - (\eta/2)\partial\phi/\partial\eta] = e^\phi.$$

In view of the result (34) for the homogeneous problem, a uniform asymptotic approximation

$$(59) \qquad \phi = -\ln(\tau_e - \tau) + \phi_0(\eta) + \mathbf{o}(1) \text{ as } \tau \uparrow \tau_e$$

is sought for η bounded. We find

$$(60) \qquad \phi_0'' - (\eta/2)\phi_0' + e^{\phi_0} = 1 \text{ where } \phi_0'(0) = 0$$

according to the symmetry condition (54); the other boundary conditions cannot be applied. But to determine ϕ_0 another boundary condition is needed and that comes from matching with the induction solution. Since ϕ_0 cannot be exponentially large, it has the asymptotic form

$$(61) \qquad \phi_0 = -2\ln\eta + A + \mathbf{o}(1) \text{ as } \eta \to \infty \text{ ,}$$

which provides the needed condition once the constant A has been determined by matching. To effect the matching we write the explicit terms (61) as functions of x and τ, and expand in $\tau_e - \tau$ to obtain

$$(62) \qquad \phi = -2 \ln x - \ln \delta + A + \mathbf{o}(1)$$

as the behavior of the induction solution as $\tau \uparrow \tau_e$ with x bounded away from zero. The numerics mentioned above do indeed exhibit such a behavior, so that $A(\delta)$ can be determined (Poland 1979, see Kassoy & Poland 1980a; Kapila 1980). The procedure fails if δ is subcritical because the numerical integration does not yield the required form (62) but tends to a steady state instead.

The expansion (59) exhibits a focussing effect in that constant values of ϕ_0 moves towards $x = 0$ as $\tau \uparrow \tau_e$, i.e. the peak of the temperature

distribution for τ constant becomes sharper as thermal runaway approached. This feature persists into the explosion phase, as we shall see shortly, so that a well-defined hot spot is formed. A combination of asymptotics and numerics therefore provides a complete picture for $\tau < \tau_e$.

Induction is immediately followed by explosion, discussed by Kassoy & Poland (1980b) and by Kapila (1980), for which the time variable (42) is appropriate. While nonlinear scalings have been encountered before in asymptotics, even in combustion (Sec. II.5), an exponential one appears to be novel. It is fundamental to the process considered here. In view of its role in thermal runaway it is not surprising that η is the other appropriate variable for the explosion phase. In terms of σ,η the governing equation becomes

$$(63) \qquad \partial T/\partial \sigma + \theta[(\eta/2)\partial T/\partial \eta - \partial^2 T/\partial \eta^2] = (T_0^2/Y_0)(H_0-T)\exp(\theta/T_0 -\theta/T -\theta\sigma).$$

Since

$$(64) \qquad x = \delta^{-1/2} \eta e^{-\theta\sigma/2},$$

the $O(1)$ values of σ and η for which the equation is valid correspond to an exponentially thin region, the hot spot, that rapidly gets thinner as time increases. The focussing as thermal runaway is approached therefore continues during the explosion stage.

If the reaction term in equation (63) is to play a role, we must write

$$(65) \qquad T = T_0/(1 - \sigma T_0) + \theta^{-1}T_1(\eta,\sigma) + o(\theta^{-1})$$

[cf. the result (43)]. The variable σ only appears as a parameter in the equation for T_1, so that its solution may be written

(66) $T_1 = T_0^2\{\psi(\eta) - \ln[(1 - T_0\sigma)(Y_0 - H_0 T_0\sigma)/Y_0]\}/(1 - T_0\sigma)^2$

where

(67) $\psi'' - (\eta/2)\psi' + e^\psi = 1$ with $\psi'(0) = 0.$

This is identical to the problem (60) for ϕ_0; indeed, matching the expansions (36) and (65) under the transformation (42) demands

(68) $\psi \equiv \phi_0.$

It follows that the boundary layer at $x = 0$ in the explosion phase is completely determined by the focussing effect in the induction phase and indeed inherits the spatial structure of that effect.

The explosion is so rapid that the temperature in the slab away from $x = 0$ stays sensibly frozen at the value

(69) $T = T_0 + \theta^{-1} T_0^2 (-2\ln x - \ln\delta + A) + o(\theta^{-1})$

attained during the induction phase. Clearly this does not match the expansion (65), even to leading order. An intermediate expansion is needed to describe the structure left behind by the rapidly shrinking hot spot. The breakdown of the approximation (69) when $\ln x = 0(\theta)$ suggests that

(70) $X = -2\theta^{-1} \ln x = \sigma - \theta^{-1} \ln(\eta^2/\delta)$

is an appropriate variable to use with σ. In fact, the intermediate expansion is independent of σ, which means that the residual structure is stationary too. Details have been given by Kapila (1980); we merely note here that the leading term $T_0/(1 - T_0 X)$ ranges between those in the expansions (65) and (69) as X decreases from σ to 0.

Within the hot spot the expansion (65) is valid until σ approaches $Y_0/H_0 T_0$, i.e. T approaches H_0. If a gaseous reactant is being considered and H_0 differs appreciably from T_0, as it often does in practice, the fluid mechanics can no longer be ignored through adoption of the constant-density approximation (Kassoy & Poland 1980b). Otherwise one continues with Kapila (1980) to subsequent phase where the time variable (45) is appropriate; that is not suggested the t̶h̶e̶ expansion (65) as far as we have taken it but by the next term. The corresponding space variable is

(71) $\qquad \xi = \delta^{1/2} \, x/\epsilon^{1/2}$

since that ensures a diffusion term in the equation

(72) $\qquad \partial\phi/\partial w - \partial^2\phi/\partial\xi^2 = -\dot\phi e^{\phi}$

governing the coefficient $T_1(\xi,w)$ in the generalization of the expansion (44). The initial condition

(73) $\qquad \phi = - \ell n(-w) - \ell n \ell n(-w) + \psi(\eta) + o(1)$ as $w \to -\infty$ with
$\qquad\qquad\qquad \eta = \xi/(-w)^{1/2}$ fixed

comes from matching with the explosion phase while the boundary condition

(74) $\qquad \phi = - \ell n \, \xi^2 - \ell n \ell n \, \xi^2 + A + o(1)$ as $\xi \to \infty$ with w fixed

comes from matching with the intermediate expansion, neither of which will be derived here; in addition

(75) $\qquad \partial\phi/\partial\xi = 0$ for $\xi = 0$.

These conditions leave the origin of w undetermined, as in the homogeneous problem, but otherwise ensure a unique solution.

Fig. 3 shows the picture which emerges from the numerical solution (Kapila 1980). Since the initial condition (73) is effectively independent of ξ when that variable is $O(1)$, the curves at first have a plateau on the left which is continually eroded by the boundary condition (74). There comes a time, however, when the erosion is stopped and the plateau begins to reestablish itself over ever-increasing distances, i.e. an incipient deflagration wave is formed. The focussing effect is then being limited by reactant depletion and the hot spot, now fast approaching the temperature H_0, begins to spread as the reaction zone detaches itself from the center and starts to propagate across the cold unburnt slab, leaving behind almost depleted reactant. Most of what was the final relaxation phase in the homogeneous problem is now taken up by this transition from hot spot to flash-through.

The remainder and more is swallowed up by the propagation phase, which takes much longer than the transition phase but is still very brief. Indeed the result (II.22) shows that, for an $O(\theta^{-1}e^{\theta/T_0})$ value of D, the deflagration wave takes a time $O(\theta\epsilon^{1/2})$ to reach the surface of the slab. This suggests using the variables

(76) $\qquad \zeta = [x_*(s) - x]/\theta\epsilon^{1/2}, \; s = (\tau - \tau_e)/\theta\epsilon^{1/2}$

to investigate the flash-through, where ζ is measured from the location x_* of the flame front. The fact that $O(\theta^{-1})$ changes in ζ measure the same distances as $O(1)$ changes in ξ, i.e. that the flame structure will be described on the scale of ξ, supports this suggestion.

To trace the progress of the deflagration wave through the intermediate region into the main part of the slab, note that the region is both

stationary and much thicker than the preheat zone of the wave. Far ahead of the flame sheet (on the scale of the preheat zone) at the instant it reaches the position X the temperature is $T_0/(1 - T_0 X)$ while everywhere behind the temperature is H_0. According to the result (II.22) the flame velociy is therefore given by

$$(77) \qquad \dot{x}_*(s) = \sqrt{2/\delta} \, H_0^2 (1 - T_0 X)/(Y_0 - H T_0 X).$$

As X decreases from $Y_0/H_0 T_0$ to zero through the intermediate region, the wave decelerates rapidly from infinity to $\sqrt{2\delta} \, H_0^2/Y_0 \theta \epsilon^{1/2}$, the velocity at which it flashes through the main part of the slab. (The flame moves more rapidly the closer the unburnt mixture is to the flame temperature H_0 because the heat of combustion is able to preheat a larger amount.)

The propagation phase ends when the preheat zone reaches the surface. In the ensuring relaxation phase the wave rapidly decelerates to zero, thereby establishing a steady state with the reaction zone just inside the slab. Details are given by Kapila (1980); we merely note that the relaxation take a very short time $O(\theta \epsilon^{3/2})$ to be completed [cf. the $O(\epsilon)$ relaxation time for the homogeneous explosion].

We do not go into details of the relaxation phase because it is a creature of the unphysical boundary condition on Y. If instead of maintaining the reactant at the surface it is prevented from diffusing across the surface, then nothing changes until the relaxation phase since $Y + T$ is constant to leading order everywhere. At that time the wave does not come to rest, but is quenched by the cold surface (Buckmaster 1979), leaving behind reactant-depleted material at temperature H_0 except for a small amount of unburnt reactant near the surface. Since the boundary continues to be

maintained at T_0, there follows a relaxation phase of duration $O(1)$
during which essentially pure heat conduction lowers the temperature
everywhere to T_0 again and the residual reactant spreads across the
slab, being slowly burnt in the process.

Our analysis describes the formation of a hot spot from which emerges
a deflagration wave that rapidly consumes the combustible material.
These are characteristics of actual explosions, so that the model has
clearly retained the essential physics. For a solid, modifications are
necessary to account for infinite Lewis number but these only change details.
For a gas, the neglect of the fluid mechanics has undoubtedly excluded
significant effect (Kassoy & Poland 1980b), in particular the evolution of
the deflagration into a detonation. The real value of the discussion,
however, lies in its elucidation of the extremely rapid transients typical
of the explosion process, one of the most challenging aspects of combustion
theory.

5. Ignition.

Thermal explosion is triggered in a combustible material by the build-up
of heat which cannot escape in sufficient amounts through the boundary.
By contrast, ignition is caused by some external source of energy. For
example, part or all of the boundary may slowly be raised to a high
temperature so that reaction starts nearby. Such a problem was considered
in Sec. 2 for a slab. (Sudden elevation of temperature is of more interest.)
Alternatively, a radiative heat flux may be applied, a mechanism that is some-
times a factor in the spread of fires.

Thermal runaway is not only a characteristic of explosion but also of ignition. As is clear from Sec. 4, if the goal is limited to calculating the time to runaway, then only the induction stage need be considered. Indeed, that is as far as the analysis has been taken by anyone to date. Our intention is not only to draw attention to ignition problems and what needs to be done (problems which only make sense in the context of large activation energy) but also to disclose another way in which runaway can occur.

The specific problem we shall examine is that of ignition of a half space by a constant energy flux (Liñán & Williams 1971). Modifications for a slab with its other surface insulated (say) are minor and will be obvious. Since the discussion does not go beyond thermal runaway, reactant depletion may be neglected; so that only the temperature equation (17) need be considered, i.e.

$$(78) \qquad \partial T/\partial t - \partial^2 T/\partial x^2 = De^{-\theta/T}$$

in the present geometry. The boundary and initial conditions are

$$(79) \quad \partial T/\partial x = T_0' > 0 \quad \text{for } x = 0, \ T = T_0 \text{ for } t = 0 \text{ and as } x \to -\infty$$

if the half-space lies in $-\infty < x \le 0$. Initially the temperature is uniform so that, in the absence of external stimulus (e.g. when the surface is insulated), there will eventually be an explosion if D is large enough. However, we are concerned with the (earlier) occurrence of runaway due to the constant heat flux applied at the boundary.

To establish some preliminary ideas define T_r, a temperature characterizing the reactivity of the material, by

(80) $$D = A(\theta)e^{\theta/T_r}$$

where $A(\theta)$ is algebraic in θ. Clearly T_r should be greater than T_0; otherwise there will be reaction from the start $(0 < T_r \leq T_0)$ or no reaction at all $(T_r < 0)$. The equation governing T is then

(81) $$\partial T/\partial t - \partial^2 T/\partial x^2 = A(\theta)\exp(\theta/T_r - \theta/T)$$

where, at times sufficiently small for T to be less than T_r everywhere, the right-hand side is negligible. The solution

(82) $$T = T_0 + T_0'[2\sqrt{t/\pi} \exp(-x^2/4t) + x \, \text{erfc} \, (|x|/2\sqrt{t})]$$

satisfying the conditions (79) increases monotonically in t but decreases monotonically in $|x|$, so that the value T_r is first attained at $x = 0$, the time being

(83) $$t_r = \pi(T_r - T_0)^2/4T_0'^2.$$

At that instant the reaction term must be reinstated. [To obtain t_r in terms of D, correct to leading order, insert $T_r = \theta/\ln D$.]

An accurate estimate of the runaway time must involve $A(\theta)$, i.e. the reaction (as in Sec. 4). Nevertheless, the notion that the temperature rises purely by heat conduction until it reaches some specific value determined by the magnitude of D, whereupon reaction becomes important enough to produce runaway within a time $O(\theta^{-1})$, is central to the development.

For times close to t_r, the reactionless solution (82) is only valid away from $x = 0$, i.e. it becomes an outer expansion. Since reaction requires T to be within $O(\theta^{-1})$ of T_r and runaway is expected to occur within a time $O(\theta^{-1})$ of t_r we introduce an inner expansion

$$(84) \qquad T = T_r + \theta^{-1}T_1(\xi,\sigma) + \theta^{-3/2}T_2(\xi,\sigma) + o(\theta^{-3/2}),$$

where

$$(85) \qquad \xi = \theta x \quad \text{and} \quad \sigma = \theta(t - t_r).$$

The choice of scale for ξ is dictated by the requirement that $\partial T_1/\partial \xi$ be $O(1)$ so as to accomodate the imposed heat flux, namely

$$(86) \qquad \partial T_1/\partial \xi = T_0' \quad \text{at} \quad \xi = 0,$$

while the term in $\theta^{-3/2}$ is induced by an intermediate expansion which must be introduced later.

The equation for T_1 is

$$(87) \qquad \partial^2 T_1/\partial \xi^2 = -\lim_{\theta \to \infty} [\theta^{-1}A(\theta)]\exp(T_1/T_r^2)$$

while $\partial^2 T_1/\partial \xi^2 = o(1)$ as $\sigma \to -\infty$ comes from matching with the solution (82). We conclude that A must be $o(\theta)$ and, in view of the condition (86), that

$$(88) \qquad T_1 = T_{10} + T_0'\xi,$$

where

$$(89) \qquad T_{10}(\sigma) = T_0'\sigma/\sqrt{\pi t_r} + o(1) \quad \text{as} \quad \sigma \to -\infty$$

but is otherwise undetermined at this stage. The equation for T_2 is

$$(90) \qquad \partial^2 T_2/\partial \xi^2 = -C \exp(T_1/T_r^2)$$

if the choice

(91) $$A = C\theta^{1/2} + o(\theta^{1/2})$$

is made, the requirement $\partial^2 T_2/\partial\xi^2 = o(1)$ as $\sigma \to -\infty$ being met for any constant C. The solution satisfying

(92) $$\partial T_2/\partial\xi = 0 \quad \text{for} \quad \xi = 0$$

has the property

(93) $$\partial T_2/\partial\xi = (CT_r^2/T_0')\exp(T_{10}/T_r^2) + o(1) \quad \text{as} \quad \xi \to -\infty,$$

which is all we shall need to know about it. So far there is no reason to suspect runaway: indeed the fact that T_{10} becomes infinite after a finite time comes from consideration of an intermediate region, to which we now turn.

The inner approximation must break down when $\xi = O(\theta^{1/2})$ since on the scale

(94) $$X = \theta^{1/2}x$$

the time derivative $\partial/\partial\sigma$ is as important as $\partial^2/\partial X^2$. The inner expansion suggest that the temperature differs from T_r by $O(\theta^{-1/2})$ there, so that we write the intermediate expansion

(95) $$T = T_r + \theta^{-1/2}T_1(X,\sigma) + \theta^{-1}T_2(X,\sigma) + o(1).$$

The equation for T_1 is

(96) $$(\partial/\partial\sigma - \partial^2/\partial X^2)T_1 = 0,$$

the temperature being too far from T_r for there to be any reaction (to any order). Matching with the inner and outer expansions and with the solution (82) require

(97) $\qquad T_1 = 0, \quad \partial T_1/\partial X = T_0' \quad$ for $\quad X = 0,$

(98) $\qquad T_1 = T_0' X + o(1) \quad$ as $\quad X \to -\infty$ and as $\quad \sigma \to -\infty.$

There is one boundary condition too many but that does not prevent there being a solution

(99) $\qquad T_1 = T_0' X.$

Continuing to T_2 yields

(100) $\qquad (\partial/\partial\sigma - \partial^2/\partial X^2)T_2 = 0,$

(101) $\qquad T_2 = T_{10}, \quad \partial T_2/\partial X = (C T_r^2/T_0') \exp(T_{10}/T_r^2) \quad$ for $\quad X = 0,$

(102) $\qquad T_2 = T_0'(X^2 + 2\sigma)/2\sqrt{\pi t_r} + o(1)$ as $X \to -\infty$ and as $\sigma \to -\infty;$

unlike that for T_1, this problem is not overdetermined since T_{10} has yet to be found. Indeed its elimination from the boundary conditions (101) gives the single nonlinear condition

(103) $\quad \partial T_2/\partial X = (C T_r^2/T_0') \exp(T_2/T_r^2)$ for $X = 0.$

All parameters can be purged by writing

(104) $\qquad \begin{cases} T_2 = T_0'(X^2 + 2\sigma)/2\sqrt{\pi t_r} + T_r^2 \widetilde{T}_2, \quad X = (\pi t_r T_r^4/T_0'^2)^{1/4}\widetilde{X}, \\[2mm] \sigma = (\pi t_r T_r^4/T_0'^2)^{1/2}[\widetilde{\sigma} + \frac{1}{4} \ln(T_0'^6/\pi t_r T_r^4 C^4)] \end{cases}$

to obtain

$$(\partial/\partial\tilde{\sigma} - \partial^2/\partial\tilde{X}^2)\tilde{T}_2 = 0,\qquad(105)$$

$$\partial\tilde{T}_2/\partial\tilde{X} = \exp(\tilde{\sigma} + \tilde{T}_2)\quad\text{for}\quad X = 0,\qquad(106)$$

$$T_2 = o(1)\quad\text{as}\quad X \to -\infty\quad\text{and as}\quad \sigma \to -\infty.\qquad(107)$$

Numerical solution of this problem shows that $\tilde{T}_2$ becomes unbounded at a definite time

$$\tilde{\sigma} = -.431\qquad(108)$$

(Liñán & Williams 1971). In terms of the original time variable, runaway therefore occurs at

$$t_r + \theta^{-1}(\pi t_r T_r^4/T_0'^2)^{1/2}[-.431 + \tfrac{1}{4}\,\ell n\,(T_0'^6/\pi t_r T_r^4 c^4)].\qquad(109)$$

The mathematical problem for runaway can therefore assume different forms. The nonlinear driving term is in the governing equation (55) and acts on $O(1)$ time and length scales. Here it is in the boundary condition (106) and acts over a time $O(\theta^{-1})$ at distances $O(\theta^{-1/2})$. Moreover the occurrence of runaway depends on the reactivity of the material in some cases but not in others. The explosion of Sec. 4 requires $T_r = T_0$ and materials of lower reactivity $(T_r > T_0)$ will never explode; on the other hand, the ignition considered here will occur for any $T_r > T_0$, as will the explosion of Sec. 3 (albeit after an exponentially long warm-up period) if T_r is also less than H_0.

6.   Explosion of Separated Reactants.

If two parallel streams, one a combustible mixture and the other
a hot inert, are allowed to come into contact then eventually the mixture will
be ignited by the inert. Such is the steady problem considered by Marble
& Adamson (1954). Here we shall treat a somewhat different problem having
some of the same features but closer to the thermal explosion investigated
in Sec. 4. Mathematically it is identical to a special case of the unsteady
mixing and explosion of two initially separated reactants considered by
Liñán & Crespo (1972). Indeed we shall retain the notation of the unsteady
problem so as to use results from Sec. 4 without translation. One feature
missing from the Marble-Adamson problem is the diffusion flame which manifests
itself as a Burke-Schuman flame sheet sufficiently far downstream.

Consider a semi-infinite flat plate (Fig. 4) separating fast parallel
streams containing oxidant X and fuel Y that come into contact at the
trailing edge and then interdiffuse to form a combustible mixture down-
stream. For simplicity the speeds, reactant concentrations and temperatures
of the streams will be taken equal. (Liñán & Crespo's problem is equivalent
to one allowing for unequal concentrations and temperatures.) For small
values of t no significant reaction occurs; for large values there is
chemical equilibrium, with a Burke-Schumann flame sheet separating a
region in which X is zero from one in which Y is zero. How the com-
bustion field evolves from the initial regime to the final one as t
increases is the main question. Such a transition arises in many combustion
processes, another example being the unsteady ignition of a fuel drop, so that
a mathematical description is of considerable interest. Moreover,
experiments have been carried out under conditions similar to those in
Fig. 4 [Liebman, Corry & Perlee (1970)].

The essential details of the combustion field can be uncovered by activation-energy asymptotics, as was shown by Liñán & Crespo (1972). Their discussion is highly intuitive since asymptotic methods were not well developed at that date, but nevertheless they accurately described the main features of their more general problem. The present discussion is more systematic and the description richer; only for the sake of simplicity is the problem specialized.

The high velocity of the streams enables longitudinal diffusion to be neglected (cf. Sec. VIII.6); in addition we adopt the constant-density approximation. Taking unit Lewis numbers then leads to the governing equations

$$(110) \qquad (\partial/\partial t - \partial^2/\partial x^2)T = -2(\partial/\partial t - \partial^2/\partial x^2)X = -2(\partial/\partial t - \partial^2/\partial x^2)Y = D(XY/Y_0^2)e^{-\theta/T}$$

if the reaction is first-order in both fuel and oxidant. Such equations, being parabolic, require only initial condition; we shall take

$$(111) \qquad T = T_0, \quad X = \begin{cases} X_0, \\ 0, \end{cases} \quad Y = \begin{cases} 0 & \text{for } x < 0 \\ Y_0 & \text{for } x > 0 \end{cases} \quad \text{at } t = 0$$

with

$$(112) \qquad X_0 = Y_0$$

to guarantee symmetry about the t-axis, a simplification that does not exclude any essential feature. The variable t is time-like, so that corresponding terminology will be adopted; when t is interpreted as time, equations (110) govern Liñán & Crespo's one-dimensional unsteady problem of two half-spaces of fuel and oxidant brought suddenly into contact at the initial instant. (Their generalization consists of different

temperatures for $x \overset{<}{\underset{>}{}} 0$ and $X_0 \neq Y_0$; they also take variable density

into account by means of the Howarth-Dorodnytsin transformation.)

The linear combinations

(113) $G = T + 2X, \quad H = T + 2Y$

satisfy pure heat equations everywhere with step functions for initial

values; whence follow the Shvab-Zeldovich relations

(114) $G = H_0 - Y_0 \text{ erf } \tilde{\eta}, \quad H = H_0 + Y_0 \text{ erf } \tilde{\eta} \quad (H_0 = T_0 + Y_0),$

where the similarity variable

(115) $\tilde{\eta} = x/2\sqrt{t}$

arises naturally. We now need only consider the temperature equation

which, in terms of t and $\tilde{\eta}$ as independent variables, becomes

(116) $t \dfrac{\partial T}{\partial t} - \dfrac{1}{2}\tilde{\eta} \dfrac{\partial T}{\partial \tilde{\eta}} - \dfrac{1}{4} \dfrac{\partial^2 T}{\partial \tilde{\eta}^2} = tD(XY/Y_0^2)e^{-\theta/T}$

where X and Y have just been determined as functions of T and $\tilde{\eta}$.

Behavior for small and large values of t can be inferred from this form

of the equation, for any value of θ, by noting that the effective

Damköhler number is tD: for t small the combustion is nearly frozen

whereas for t large it is near equilibrium.

In the limit $t \to 0$ we find

(117) $T = T_0, \quad X = Y_0(1 - \text{erf } \tilde{\eta})/2, \quad Y = Y_0(1 + \text{erf } \tilde{\eta})/2.$

At any finite value of x when t is small there is a combustible

mixture, formed by interdiffusion of the reactants, in which no

significant reaction has taken place. We may therefore expect a thermal

explosion similar in many respects to the spatially inhomogeneous one discussed in Sec. 4.

In the limit $t \to \infty$ we must have

(118) $XY = 0$

and then the relations (114) show that

(119) $T = \begin{cases} H_0 + Y_0 \text{ erf } \tilde{\eta}, \\ H_0 - Y_0 \text{ erf } \tilde{\eta}, \end{cases}$ $X = \begin{cases} -Y_0 \text{erf } \tilde{\eta} \\ 0 \end{cases}$, $Y = \begin{cases} 0 & \text{for } x < 0, \\ Y_0 \text{ erf } \tilde{\eta} & \text{for } x > 0. \end{cases}$

There is a Burke-Schumann flame sheet, corresponding to infinite Damköhler number (cf. Sec. VI.2), located on the t-axis at a temperature

(120) $T_* = H_0.$

On the scale of $\tilde{\eta}$ the flame sheet is a discontinuity so that, to investigate its structure, we introduce the variables

(121) $\zeta = t^{1/3}\tilde{\eta} = x/2t^{1/6}$, $\Theta = \sqrt{\pi} t^{1/3}(T_* - T)/2Y_0$

and seek a solution for which Θ is a function of ζ alone. This choice of variables ensures a meaningful balance of diffusion and reaction, i.e. a distinguished limit of equation (116) in asymptotic parlance. The limit is

(122) $d^2\Theta/d\zeta^2 = c(\Theta^2 - \zeta^2)$ with $c = 2De^{-\theta/H_0}/\sqrt{\pi Y_0}$

and matching with the outer solutions (119) requires the boundary conditions

(123) $d\Theta/d\zeta = \pm 1 + o(1)$ as $\zeta \to \pm\infty$.

The problem (122,123) is that for the classical Burke-Schumann structure (cf. Sec. VI.2).

The evolution from the frozen regime to the equilibrium regime turns out to be remarkably simple in the limit $\theta \to \infty$. Thermal runaway occurs in the diffusion-generated mixture at a point on the line of symmetry and a hot spot develops just as for the spatially inhomogeneous explosion of Sec. 4. As the temperature in the hot spot approaches its ultimate value H_0 (corresponding to complete consumption of the reactants) a symmetrical pair of deflagration waves is formed, which penetrate the large temperature gradients left behind by the focussing hot spot and flash through the layers of frozen mixture consuming all of the deficient reactant. All this happens within a range of t (including the runaway point) that is exponentially smaller than the scale of mixing.

A detailed description starts with the induction phase, during which the temperature rises from the initial value T_0 by only an $O(\theta^{-1})$ amount. The corresponding small-disturbance equation

$$(124) \qquad \partial\phi/\partial t - \partial^2\phi/\partial x^2 = \delta(1 - \mathrm{erf}^2\tilde{\eta})e^{\phi}$$

differs from that (55) for an initially uniform slab only in having an extra factor on the righthand side; if we now restrict the discussion to the region $x > 0$, the boundary conditions

$$(125) \qquad \partial\phi/\partial x = 0 \;\text{ for }\; x = 0, \;\; \phi = 0 \;\text{ for }\; t = 0$$

are the same. As there the solution becomes unbounded at a point

$$(126) \qquad \tau = \tau_e \;\text{ on }\; x = 0$$

which can be determined numerically (Liñán & Crespo, 1972).

The behavior of ϕ as $\tau \to \tau_e$ is given by equation (59) since $\tilde{\eta}$ is $O(\tau_e - \tau)^{1/2}$ in the variables τ and η. The function ϕ_0 is changed because the constant A in its asymptotic expansion (61) is different, being determined by the asymptotic form (62) of the solution to a different problem. (The value of A has never been computed.)

The explosion phase is governed by the equation (63) with right-hand side replaced by

$$(127) \qquad (T_0^2/4Y_0^2)(H_0-T)^2 \exp(\theta/T_0 - \theta/T - \theta\sigma)$$

since $\tilde{\eta}$ is effectively zero there. The reactant concentrations are changed from $Y_0/2$ to zero as T increases from T_0 to H_0. The expansion (65) is still valid, but now

$$(128) \qquad T_1 = T_0^2\{\psi(\eta) - 2\ln[(Y_0 - H_0T_0\sigma)/2Y_0]\}/(1 - T_0\sigma)^2$$

where again ψ satisfies the equation (67) and hence the identity (68) with the new ϕ_0. Between the hot spot described by this expansion and the essentially frozen combustion field on either side there is a stationary intermediate structure on the scale (70), the leading term of which is again $T_0/(1 - T_0\chi)$.

The transition phase which follows is governed by the modification

$$(129) \qquad \partial\phi/\partial\omega - \partial^2\phi/\partial\xi^2 = -\phi^2 e^\phi$$

of the equation (72), provided the definition (46) is replaced by

$$(130) \qquad \epsilon = (4Y_0^2\theta^2/H_0^2T_0^2)\exp(-\theta Y_0/H_0T_0).$$

The modification arises because the hot spot contains the reactants in stoichiometric proportion, which results in a truly second-order reaction

rather than an essentially first-order one. The initial condition (73) is replaced by

(131) $\phi = -\ln(-\omega) - 2\ln\ln(-\omega) + \psi(\eta) + o(1)$ as $\omega \to -\infty$

with $\eta = \xi/(-\omega)^{1/2}$ fixed

. while the boundary condition (74) is replaced by

(132) $\phi = -\ln\xi^2 - 2\ln\ln\xi^2 + A + O(1)$ as $\xi \to \infty$ with ω fixed.

It appears that no numerical investigation of the problem (129, 131, 132) has yet been undertaken, but similarity to the problem (72,73,74) leaves little doubt that it would yield a transition from a focussing hot spot to an incipient deflagration wave.

The wave must first traverse the intermediate structure left by the shrinking hot spot. The situation is the same as that in Sec. 4 except that ahead there is a mixture of fuel and oxidant in stoichiometric proportion, i.e. $X = Y$ [cf. equations (114) with $\tilde{\eta} = 0$]; instead of a single reactant. It follows that the variables (76) are again appropriate, if the new definition (130) of ϵ is used, but that the velocity (77 bis) must be replaced by

(133) $W = \sqrt{\delta} \dfrac{H_0^3 T_0}{Y_0 \theta^2} \exp(Y_0 \theta/2H_0 T_0)\left(\dfrac{1 - T_0 X}{Y_0 - H_0 T_0 X}\right)$

in accordance with the result (II.52). As X decreases from $Y_0/H_0 T_0$ to zero through the intermediate region the wave decelerates rapidly from infinity to

(134) $W = \sqrt{\delta}(H_0^3 T_0/Y_0^2 \theta^2)\exp(Y_0 \theta/2H_0 T_0),$

the velocity with which it enters the near-frozen external field.

For the slab considered in Sec. 4, the wave then continues at the same speed to the surface, but here it encounters non-uniformities in available enthalpy which produces $O(1)$ changes in its temperature and hence exponentially large changes in its velocity. These non-uniformities have been formed by interdiffusion of the reactants up to $t_e = \tau_e/\delta$, i.e.

$$(135) \qquad T = T_0, \quad X = Y_0(1 - \mathrm{erf}\, \tilde{\eta}_e)/2, \quad Y = Y_0(1 + \mathrm{erf}\, \tilde{\eta}_e)/2$$

where

$$(136) \qquad \tilde{\eta}_e = x/2\sqrt{t_e},$$

and have no time to change during transit of the wave.

The situation is similar to that in the intermediate region: the combustion field is stationary and has a much larger scale than that of the preheat zone of the flame. Far ahead of the wave on the latter scale the temperature and mass fractions have the distributions (135) at the instant the wave reaches the position x; while behind

$$(137) \qquad T = H_0 - Y_0\, \mathrm{erf}\, \tilde{\eta}_e, \quad X = 0, \quad Y = Y_0\, \mathrm{erf}\, \tilde{\eta}_e \text{ for } x > 0.$$

To determine the velocity of the wave we use the result (II.51) which, as was pointed out there, holds both near and far from stoichiometry. Thus

$$(138) \quad W = \sqrt{\delta}(T_0/Y_0^2\theta^2)(1-\mathrm{erf}\tilde{\eta}_e)^{-1}(H_0-Y_0\mathrm{erf}\tilde{\eta}_e)[(H_0-Y_0\mathrm{erf}\tilde{\eta}_e)^2+\theta Y_0\mathrm{erf}\tilde{\eta}_e]^{1/2}e^{\alpha\theta}$$

where

$$(139) \qquad \alpha = Y_0(1 - \mathrm{erf}\, \tilde{\eta}_e)/2T_0(H_0-Y_0\, \mathrm{erf}\, \tilde{\eta}_e)$$

is the wave speed, which clearly reduces to the value (134) for $\tilde{\eta}_e = 0$.

The result cannot be valid as $\tilde{\eta}_e \to \infty$ since the propagation is then

associated with significant changes in t; well before then, however, the

formula (II.51) fails because J_s (i.e. the oxidant flux) becomes small.

The correct result has not yet been obtained, perhaps because it would

add very little to the picture. Note that equilibrium with a Burke-

Schumann flame sheet holds at any finite x immediately after the explo-

sion: the combustion field (137) is precisely of the ultimate form (119b).

The picutre which has emerged is remarkably simple, consisting of

regions of frozen chemistry and equilibrium with reaction zones between

them, the hallmark of activation-energy asymptotics. To secure the

essential features very little analysis was required beyond that for

the thermal explosion of Sec. 4.

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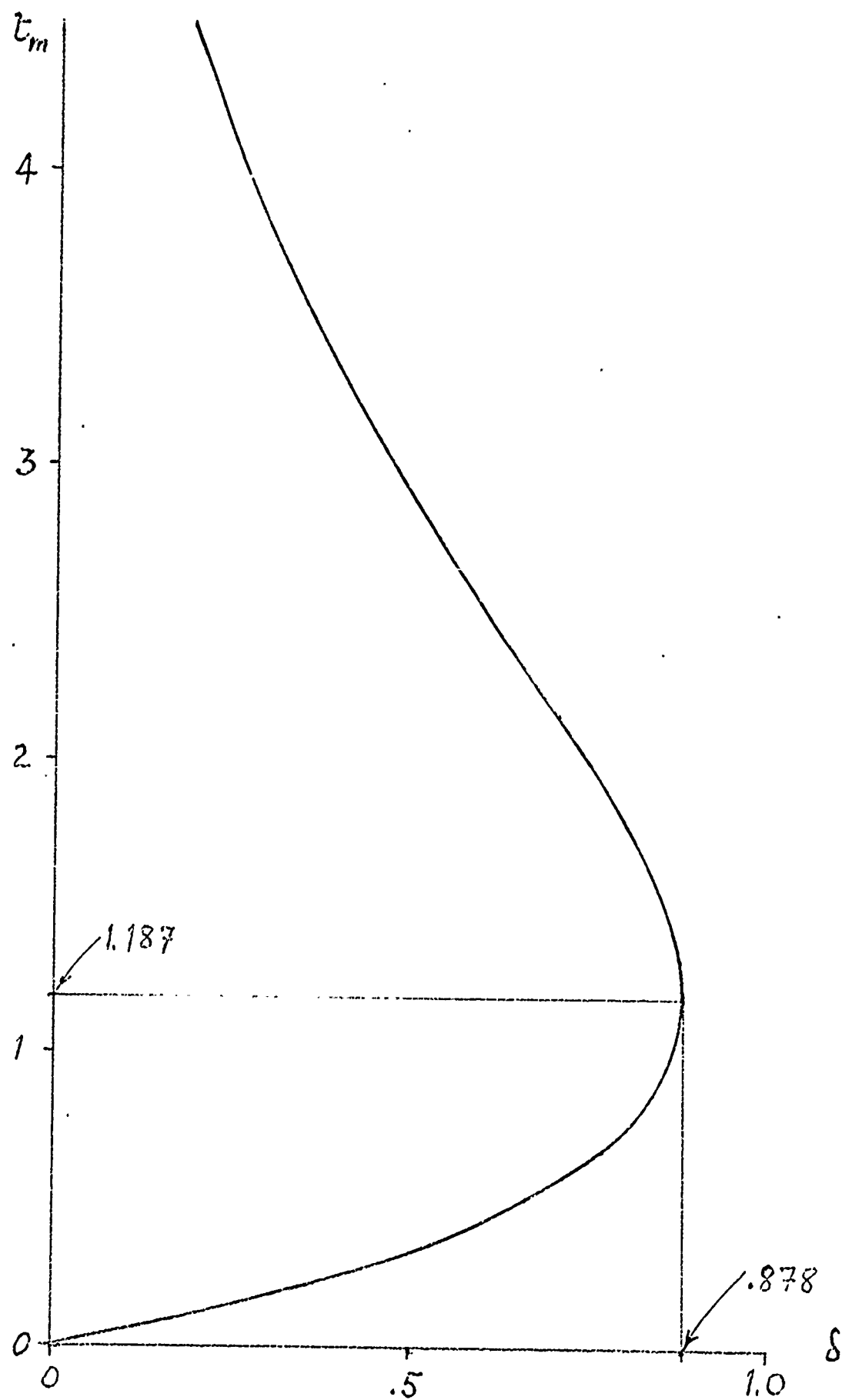   methane-air systems, Combust. Sci. Tech. 1, 257-267.
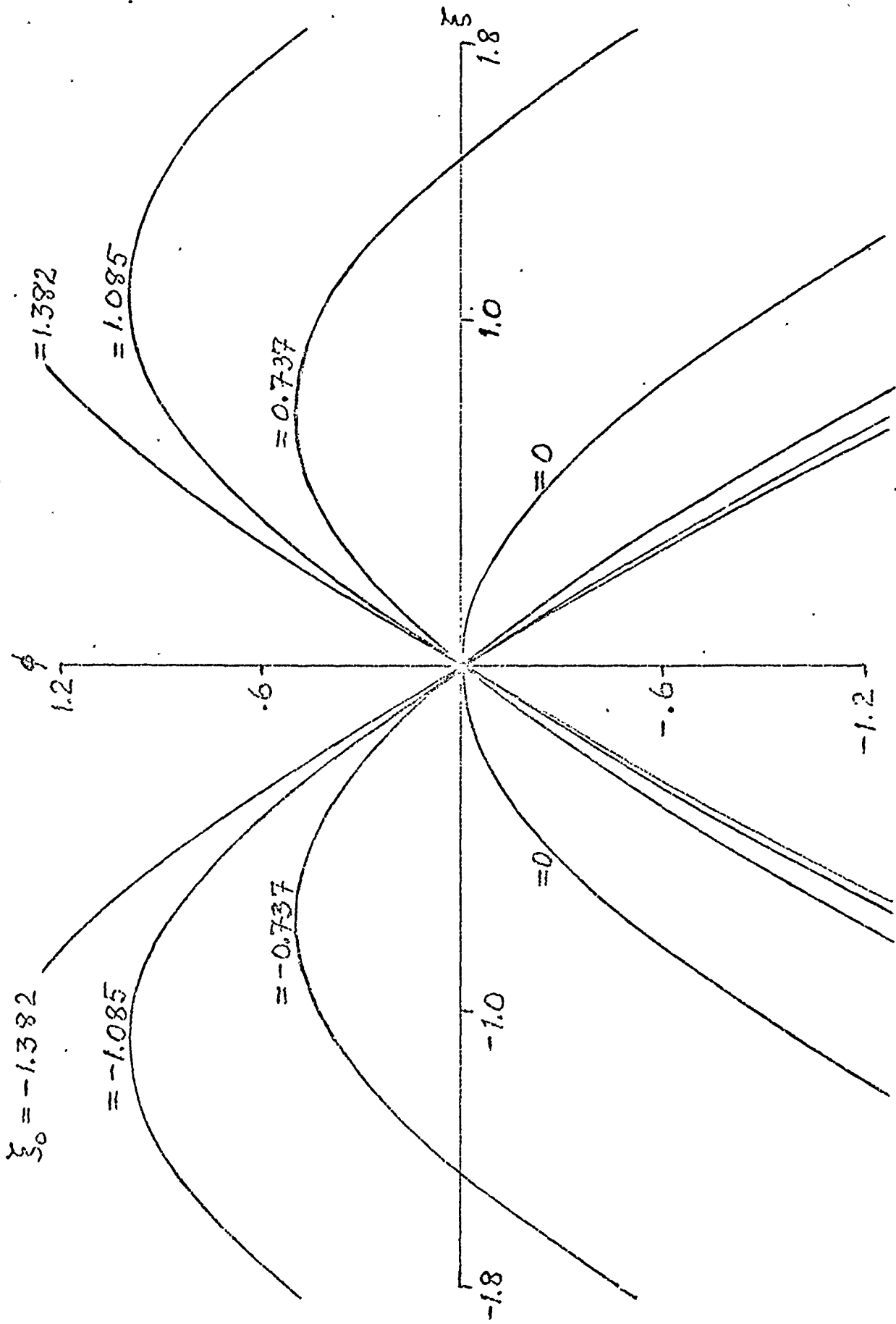
Fig.1: Response for symmetrically heated slab.

Fig. 2a: Perturbation temperature profiles in asymmetrically heated sinh's, drawn for $1-\alpha \cdot 4T_0$. Curves correspond to $\phi_o = 0(0.5)1.5$.
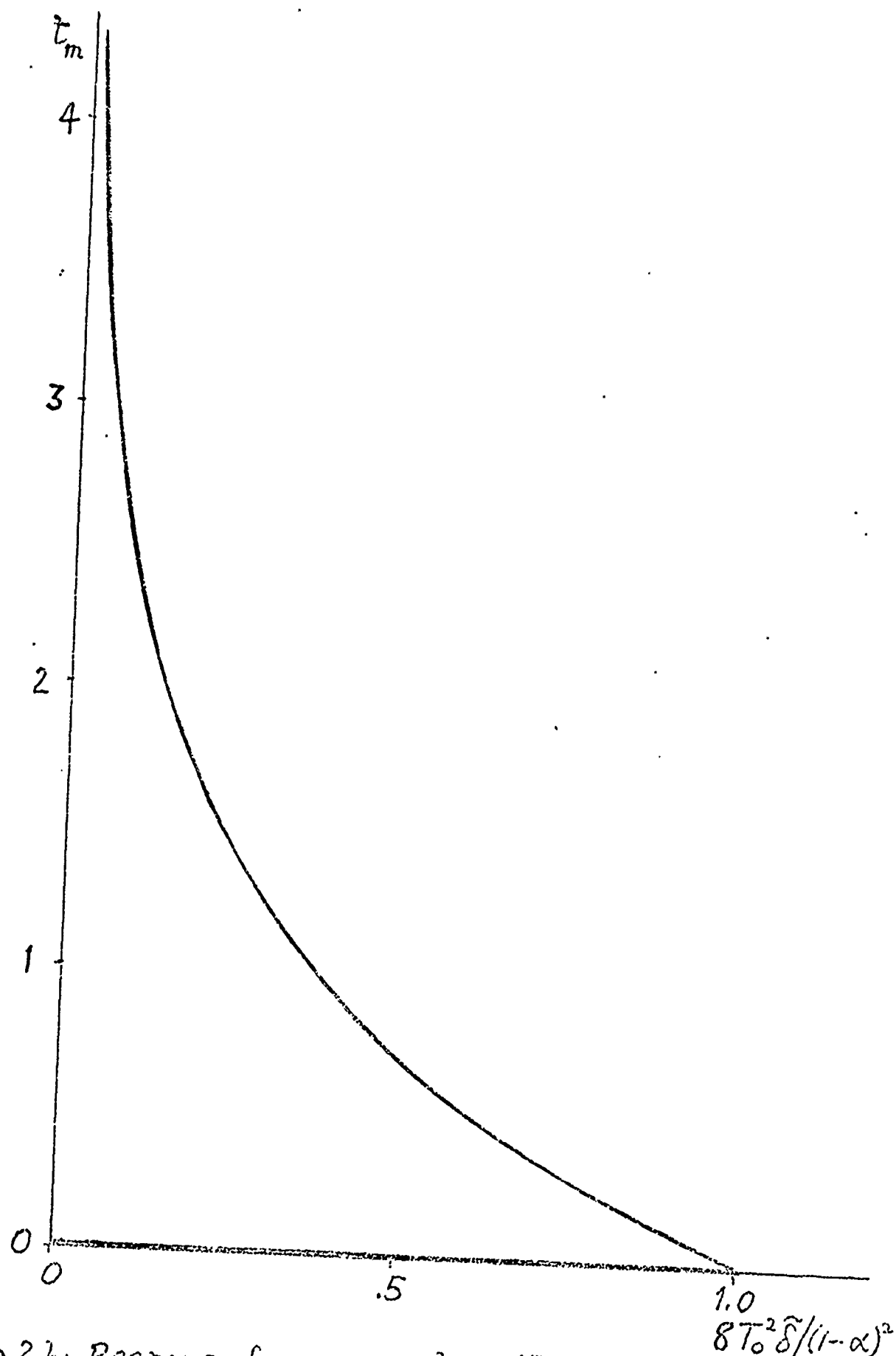
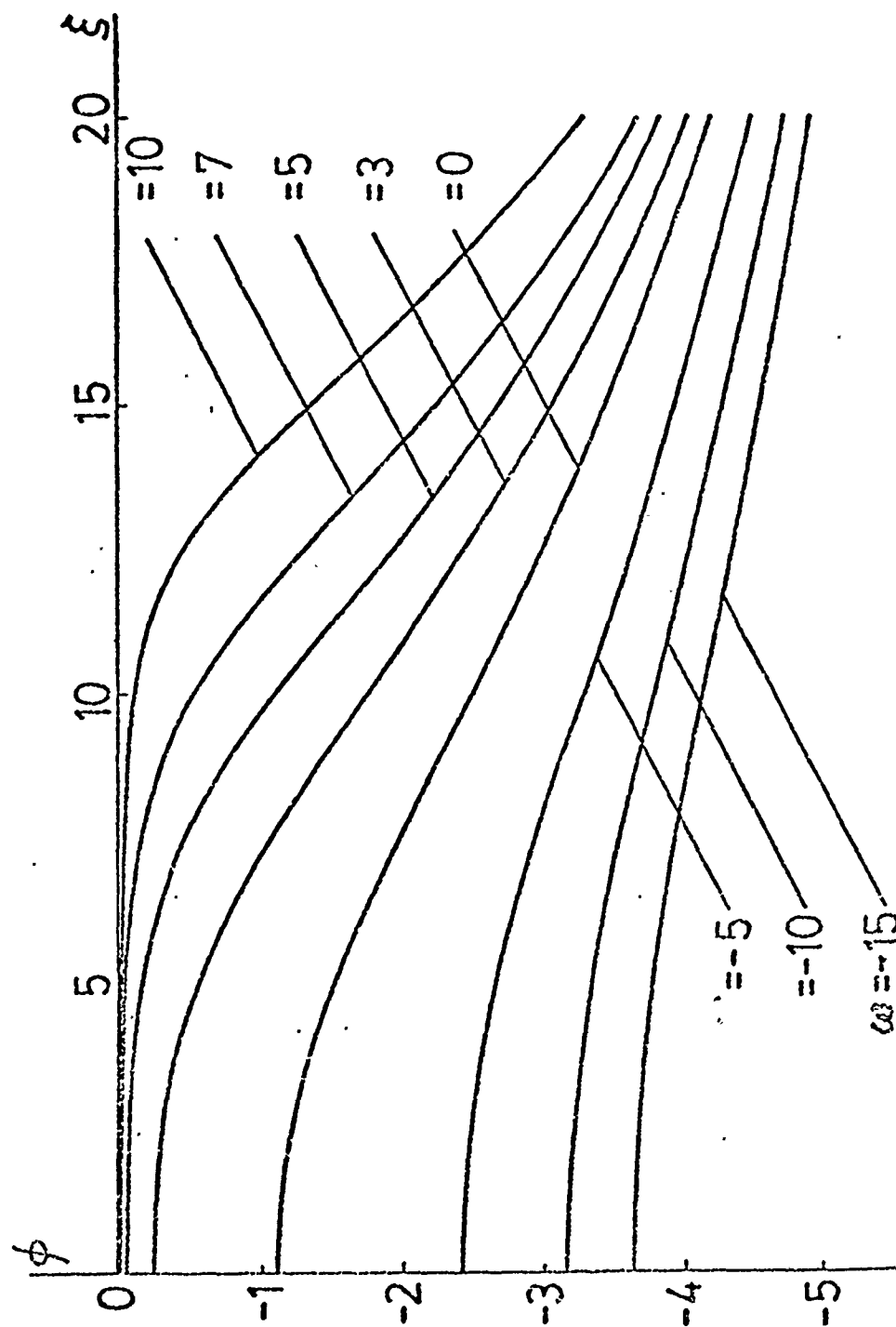Fig 2 b: Response for asymmetrically heated slab.
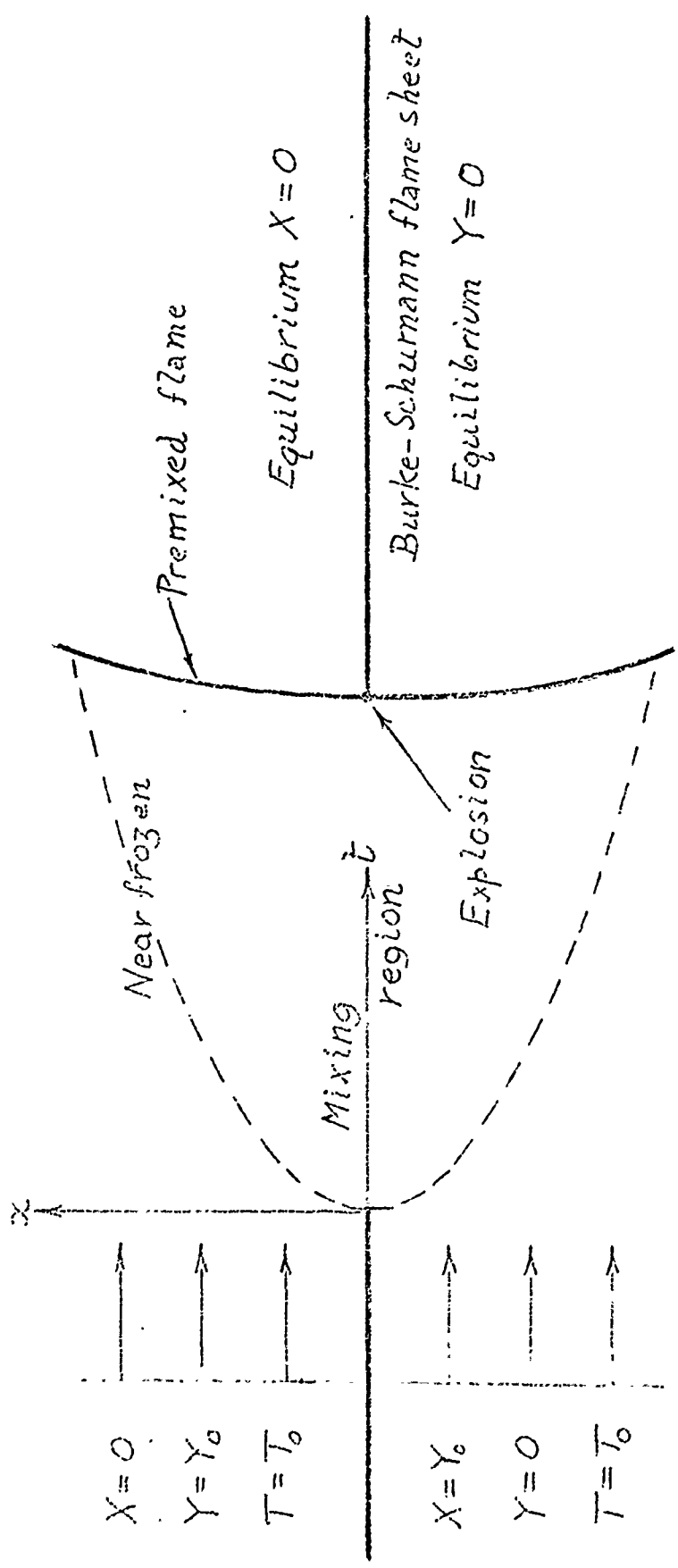
Fig.3: Transition phase: focussing to deflagration.

Fig. 4: *Combustion of initially separated reactants.*

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
114	AD-A083 549	

4. TITLE (and Subtitle)	5. TYPE OF REPORT & PERIOD COVERED
MATHEMATICAL THEORY OF LAMINAR COMBUSTION XII: Ignition and Explosion	Interim Technical Report
	6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s)	8. CONTRACT OR GRANT NUMBER(s)
J.D. Buckmaster & G.S.S. Ludford	DAAG29-79-C-0121

9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
Dept. of Theoretical and Applied Mechanics Cornell University, Ithaca, NY 14853	P-15882-M

11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE
U. S. Army Research Office	March, 1980
Post Office Box 12211	13. NUMBER OF PAGES
Research Triangle Park, NC 27709	47

14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)	15. SECURITY CLASS. (of this report)
	Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE NA

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

The findings in this report are not to be construed as an official Department of the Army position, unless so designated by other authorized documents.

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

Ignition, explosion, spontaneous combustion, thermal theory, Frank-Kamenetskii, thermal runaway, induction, relaxation, transition, propagation, subcritical, supercritical, separated reactants, hot spot, flash-through.

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

This report is Chapter XII of the twelve in a forthcoming research monograph on the mathematical theory of laminar combustion. The induction, explosion, transition, propagation and relaxation phases are described for a slab of reactant whose faces are kept at a constant temperature. Under ignition, the application of a heat flux to a half space is considered. Finally, the explosion of initially separated reactants after they have mixed is shown to be very similar to the explosion of premixed reactants.

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