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IGNITION OF A COMBUSTIBLE SOLID WITH REACTANT CONSUMPTION*

D. GLENN LASSEIGNE† AND W. E. OLMSTEAD‡

Abstract. The effects of excessive reactant consumption on the ignition of a combustible solid are introduced through a revised scaling of the heat release constant. Large activation energy asymptotics then yields a new one-parameter integral equation governing the temperature evolution near ignition. Analysis of the integral equation reveals a critical value of the parameter which distinguishes between the cases of ignition and nonignition.

Key words. ignition, reactant consumption, integral equations

AMS(MOS) subject classifications. 45G05, 80A30

1. Introduction. The purpose of this paper is twofold: first, to derive an integral equation which accounts for the effect of reactant consumption during the ignition of a combustible solid; second, to determine the properties of the solution to that integral equation so as to establish a criterion for nonignition due to excessive consumption of the reactant.

Liñan and Williams [1] first employed an asymptotic approach based upon large activation energy to derive an integral equation governing the ignition of a reactive solid. More recent work by Kapila [2], Olmstead [3] and Lasseigne and Olmstead [4] has extended and generalized the results of [1]. The assumed scaling of the parameters in [1]-[4] has been such that the amount of reactant remains constant (at least asymptotically to leading order) while thermal runaway progresses. Thus, even for a significant generalization of the problem as in [3], it is found that the Liñan-Williams integral equation emerges as the appropriate description of the transition stage leading to ignition. The inherent mathematical feature of this integral equation is that its solution becomes unbounded at finite time, thereby signalling the achievement of ignition.

In order to have enough reactant consumed to inhibit ignition, it is necessary to introduce a different scaling of the parameters than that used in [1]-[4]. Under this adjusted scaling, it will be shown that large activation energy asymptotics yields a one-parameter integral equation which is new to ignition theory. Analysis of this integral equation will reveal that its solution dramatically changes character at a critical value of the parameter. Below the critical value, the solution has a singularity analogous to that of the Liñan-Williams equation. Above the critical value no such singularity exists, which indicates that most of the reactant has been consumed without producing sufficient heat to sustain a thermal runaway.

As in [1]-[4], the physical problem is modelled by a semi-infinite solid $x \geq 0$, with external heating at the surface $x = 0$. A generalized statement of the problem similar to that given in [3] is used here. In nondimensional form, the temperature $\theta(x, t)$ of the combustible solid and the mass fraction of unexpended reactant $Y(x, t)$ satisfy

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the system

$$(1.1) \quad \theta_t = \theta_{xx} + BAY^N \exp(-E/\theta), \quad x > 0, \quad t > 0,$$

$$(1.2) \quad Y_t = -AY^N \exp(-E/\theta), \quad x > 0, \quad t > 0,$$

$$(1.3) \quad \theta_x(0, t) = \alpha\theta(0, t) - h(t), \quad \theta(\infty, t) = \theta_0, \quad t > 0,$$

$$(1.4) \quad \theta(x, 0) = \theta_0, \quad Y(x, 0) = 1, \quad x \geq 0.$$

The temperature has been normalized by a critical value θ'_c to be defined later, and $\theta_0 > 0$ is the normalized initial temperature. The mass fraction has been normalized by its initial value. The exponential term represents an N th order Arrhenius-type chemical reaction. The nondimensional parameters, A , B , E and α are all nonnegative, and they denote the Damköhler number, heat release parameter, activation energy and convection coefficient, respectively. The given function $h(t)$ can be interpreted either as an imposed heat flux at the surface $x = 0$, or as $\alpha\theta_s$, where $\theta_s(t)$ is the temperature of the medium in contact with the combustible solid.

In (1.2) the spatial diffusion of reactant has been neglected. The justification for this is that the Lewis number for combustible solids is essentially infinite. This simplification has been used by Kassoy and Poland [5], as well as in [4].

The parameters A , B and E have been introduced here in a slightly different manner than in [1]–[4]. The dimensional activation energy E' has been normalized so that

$$(1.5) \quad E = E'/R'\theta'_c \gg 1,$$

where R' is the gas constant and θ'_c is the critical temperature defined by the relationship

$$(1.6) \quad A = E e^E = \frac{E'}{R'\theta'_c} \exp\left(\frac{E'}{R'\theta'_c}\right).$$

The definitions of A and B have made so that the heat release parameter B appears multiplicatively in (1.1) and its scaling is of the form

$$(1.7) \quad B = B_0 E^{-1/2} = B_0 \left(\frac{R'\theta'_c}{E'}\right)^{1/2},$$

where B_0 is assumed to be of order unity with respect to E . It is the relative smallness of B which allows for reactant consumption to inhibit ignition. This is in contrast to the assumption that B is of order unity as used in [1]–[4].

The scalings of A and B introduced in (1.6) and (1.7) are not the only ones which lead to the results obtained in this investigation. In § 4, more general scalings will be discussed which yield similar results while allowing for a broader interpretation of the physical parameters. No specific scaling of the parameter α has been introduced here. Its size only affects the overall time scale of the problem as will be pointed out later.

2. Large activation energy asymptotics. The largeness of E motivates the choice of the small parameter

$$(2.1) \quad \varepsilon = E^{-1} \ll 1,$$

which will be used in the asymptotic analysis of (1.1)–(1.4). It is then clear that the quantity

$$(2.2) \quad A \exp(-E/\theta) = \varepsilon^{-1} \exp\left[\frac{1}{\varepsilon}(1 - \theta^{-1})\right]$$

undergoes an abrupt change of magnitude in some neighborhood of $\theta = 1$. To insure that the system (1.1)–(1.4) starts below this critical level, it will be assumed that

$$(2.3) \quad 1 - \theta_0 \gg \varepsilon.$$

The implication of (2.3) is that there exists a time interval in which the reaction term in (1.1) and (1.2) is exponentially small. During this inert stage,

$$(2.4) \quad \theta(x, t) = \theta_I(x, t) + \text{e.s.t.}, \quad Y(x, t) = 1 + \text{e.s.t.},$$

where e.s.t. signifies terms that are exponentially small in ε , and

$$(2.5) \quad \theta_I(x, t) = \theta_0 + \int_0^t G_\alpha(x, t-s)[h(s) - \alpha\theta_0] ds.$$

Here $G_\alpha(x, t)$ is the Green's function for the heat equation with a homogeneous boundary condition of the form of (1.3), so that

$$(2.6) \quad G_\alpha(x, t) = \frac{e^{-x^2/4t}}{(\pi t)^{1/2}} - \alpha e^{\alpha x + \alpha^2 t} \operatorname{erfc} \left[\frac{x}{2t^{1/2}} + \alpha t^{1/2} \right] \geq 0.$$

The inert stage results (2.4) cease to be valid as θ nears unity. Since θ_I attains its maximum value at $x = 0$, an appropriate choice for the critical time t_c near which the reaction term becomes significant is given implicitly by

$$(2.7) \quad 1 = \theta_I(0, t_c) = \theta_0 e^{\alpha^2 t_c} \operatorname{erfc}(\alpha t_c^{1/2}) + \int_0^{t_c} G_\alpha(0, t_c - s)h(s) ds.$$

It is assumed here that there exists a $t_c > 0$ that satisfies (2.7); and, if there is more than one, the minimum value is used. In [4] it has been demonstrated that, to allow for various extreme cases of physical interest, the critical time t_c need not necessarily be of order unity in ε . Thus it is appropriate to consider

$$(2.8) \quad t_c = \varepsilon^k t_0,$$

where t_0 is $O(1)$ with respect to ε . Here k may be positive, negative or zero, and it is clearly linked to whatever scaling is specified for α .

Following the inert stage is the transition stage where the reaction term is no longer exponentially small. Since the reaction term first becomes significant near $(x, t) = (0, t_c)$, it is appropriate to introduce new independent variables

$$(2.9) \quad x = \varepsilon \xi, \quad t = t_c + \varepsilon \tau = \varepsilon^k t_0 + \varepsilon \tau,$$

where, for the proper ordering of the time scale, it must be assumed that

$$(2.10) \quad k < 1.$$

The scaling of τ is crucial to the effect of reactant consumption. In terms of this stretched time, (1.2) can be expressed as

$$(2.11) \quad Y_\tau = -Y^N \exp \left[\frac{1}{\varepsilon} (1 - \theta^{-1}) \right], \quad \xi > 0, \quad \tau > -\infty$$

with the initial condition

$$(2.12) \quad Y \rightarrow 1 \quad \text{as } \tau \rightarrow -\infty.$$

Integration of (2.11) gives

$$(2.13) \quad Y = \begin{cases} e^{-v}, & N = 1, \\ [1 + (N-1)v]^{-1/(N-1)}, & N > 1, \end{cases}$$

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where

$$(2.14) \quad v(\xi, \tau; \varepsilon) = \int_{-\infty}^{\tau} \exp \left[\frac{1}{\varepsilon} (1 - \theta^{-1}) \right] d\tau'.$$

Only the cases of $N \geq 1$ are considered since they represent those of most physical interest.

Using (2.13) in (1.1) provides a simplification of the problem to one involving only θ as a dependent variable. It is then assumed that θ has an inner asymptotic expansion (valid in the reaction zone near $x = 0$) of the form

$$(2.15) \quad \theta = \theta_I(\varepsilon\xi, t_c + \varepsilon\tau) + \varepsilon\phi_0(\xi, \tau) + \varepsilon^{3/2}\phi_1(\xi, \tau) + \dots.$$

By expansion of θ_I , (2.15) can be expressed as

$$(2.16) \quad \theta = 1 + \varepsilon[a\tau - b\xi + \phi_0(\xi, \tau)] + \varepsilon^{3/2}\phi_1(\xi, \tau) + \dots,$$

where

$$(2.17) \quad a = \lim_{\varepsilon \rightarrow 0} \left[\frac{\partial \theta_I}{\partial t}(0, t_c) \right], \quad b = -\lim_{\varepsilon \rightarrow 0} \left[\frac{\partial \theta_I}{\partial x}(0, t_c) \right].$$

For the success of the perturbation scheme, it is required that these limits exist and that

$$(2.18) \quad a > 0, \quad b > 0.$$

The need for these conditions and their physical implications have been discussed in [3].

The arguments leading to the determination of ϕ_0 and ϕ_1 are analogous to those of [1]-[4]. It follows from (1.1)-(1.4) that to $O(\varepsilon)$ as $\varepsilon \rightarrow 0$,

$$(2.19) \quad \frac{\partial^2 \phi_0}{\partial \xi^2}(\xi, \tau) = 0, \quad \frac{\partial \phi_0}{\partial \xi}(0, \tau) = 0, \quad \phi_0(\xi, -\infty) = 0.$$

The solution of (2.19) is

$$(2.20) \quad \phi_0(\xi, \tau) = f_0(\tau), \quad f_0(-\infty) = 0.$$

Utilizing (2.16) and (2.20) in (2.13) and (2.14) yields as $\varepsilon \rightarrow 0$,

$$(2.21) \quad Y = Y_0 + o(1), \quad Y_0(\xi, \tau) = Y|_{v=v_0},$$

where

$$(2.22) \quad v_0(\xi, \tau) = e^{-b\xi} \int_{-\infty}^{\tau} e^{a\tau' + f_0(\tau')} d\tau'.$$

Then for $O(\varepsilon^{3/2})$ as $\varepsilon \rightarrow 0$ in the perturbation scheme, it follows that

$$(2.23) \quad \frac{\partial^2 \phi_1}{\partial \xi^2}(\xi, \tau) = -B_0 Y_0^N e^{-b\xi + a\tau + f_0(\tau)}, \quad \frac{\partial \phi_1}{\partial \xi}(0, \tau) = 0, \quad \phi_1(\xi, -\infty) = 0.$$

The solution of (2.23) can be expressed as

$$(2.24) \quad \phi_1(\xi, \tau) = -B_0 e^{a\tau + f_0(\tau)} \int_0^{\xi} \int_0^{\xi'} Y_0^N(\xi'', \tau) e^{-b\xi''} d\xi'' d\xi' + f_1(\tau), \quad f_1(-\infty) = 0.$$

Since ϕ_0 and ϕ_1 constitute part of the inner expansion, no condition at $\xi = \infty$ has been prescribed. Thus f_0 and f_1 remain undetermined until a matching with an appropriate outer solution can be made.

To obtain the desired outer asymptotic solution (away from the reaction zone), a new spatial scaling is introduced as

$$(2.25) \quad \xi = \varepsilon^{-1/2} X.$$

It is then assumed that θ has an outer expansion of the form

$$(2.26) \quad \theta = \theta_I(\varepsilon^{1/2} X, t_c + \varepsilon \tau) + \varepsilon \Phi_0(X, \tau) + \dots$$

In terms of this new spatial scaling it is easily verified that the reaction term is exponentially small with respect to ε . It then follows that to $O(\varepsilon)$ as $\varepsilon \rightarrow 0$,

$$(2.27) \quad \left(\frac{\partial}{\partial \tau} - \frac{\partial^2}{\partial X^2} \right) \Phi_0(X, \tau) = 0, \quad \Phi_0(\infty, \tau) = 0, \quad \Phi_0(X, -\infty) = 0.$$

Using the Green's function (2.6), an integral representation of the solution to (2.27) can be expressed as

$$(2.28) \quad \Phi_0(X, \tau) = \int_{-\infty}^{\tau} G_0(X, \tau - \sigma) \left[-\frac{\partial \Phi_0}{\partial X}(0, \sigma) \right] d\sigma.$$

The determination of Φ_0 still necessitates some boundary condition at $X = 0$. This will be derived through a matching with the inner solution.

The matching of the inner and outer solution is achieved by considering $X \rightarrow 0$ and $\xi \rightarrow \infty$ in the equality

$$(2.29) \quad \varepsilon \Phi_0(X, \tau) + \dots = \varepsilon \phi_0(\xi, \tau) + \varepsilon^{3/2} \phi_1(\xi, \tau) + \dots$$

It follows that

$$(2.30) \quad \Phi_0(0, \tau) = f_0(\tau),$$

and

$$(2.31) \quad \frac{\partial \Phi_0}{\partial X}(0, \tau) = -\frac{B_0}{b} e^{f_0(\tau) + a\tau} F_N \left(\int_{-\infty}^{\tau} e^{f_0(\sigma) + a\sigma} d\sigma \right),$$

where

$$(2.32) \quad F_N(r) = \frac{1}{r} \begin{cases} 1 - e^{-r}, & N = 1, \\ 1 - [1 + (N - 1)r]^{-1/(N-1)}, & N > 1. \end{cases}$$

Thus an evaluation of (2.28) at $X = 0$, together with (2.30) and (2.31), yields the integral equation

$$(2.33) \quad f_0(\tau) = \frac{B_0}{b} \int_{-\infty}^{\tau} \frac{e^{f_0(\sigma) + a\sigma}}{\sqrt{\pi(\tau - \sigma)}} F_N \left(\int_{-\infty}^{\sigma} e^{f_0(\sigma') + a\sigma'} d\sigma' \right) d\sigma.$$

Since f_0 is the leading order perturbation of the temperature in the reaction zone, its properties reflect the evolution toward ignition. The Liñan-Williams equation, as derived in [1], corresponds to $F_N \equiv 1$. In that case f_0 become unbounded at a finite value of τ , which implies a thermal runaway associated with the achievement of ignition. This new integral equation (2.33) accounts for reactant consumption through the appearance of F_N . In the analysis of this equation to follow, a criterion will be established which distinguishes the case in which f_0 becomes unbounded at some $\tau^* < \infty$ from that case in which f_0 is bounded for all finite τ . The physical interpretation of this latter case is that there has been sufficient reactant consumption to inhibit ignition.

3. Analysis of the integral equation. The integral equation (2.33) governs the perturbation of temperature in the reaction zone. To analyze its properties, it is expedient to introduce the change of variable,

$$(3.1) \quad \eta = a\tau + \log(B_0/b\sqrt{a}), \quad u(\eta) = f_0(\tau).$$

This converts (2.33) to the form

$$(3.2) \quad u(\eta) = \int_{-\infty}^{\eta} \frac{e^{u(\xi)+\xi}}{\sqrt{\pi(\eta-\xi)}} F_N \left(\lambda \int_{-\infty}^{\xi} e^{u(\xi')+\xi'} d\xi' \right) d\xi, \quad \eta > -\infty,$$

where F_N is given by (2.32) and

$$(3.3) \quad \lambda = b/B_0\sqrt{a} \geq 0.$$

For a given reaction order $N \geq 1$, the solution of (3.2) depends only on the parameter λ . This parameter reflects the influence of inert heating through the appearance of a and b , while B_0 reflects the influence of the exothermicity of the reaction. From a physical viewpoint, it is convenient to think of $\lambda \ll 1$ as a hot reaction with sufficient reactant, and $\lambda \gg 1$ as either a cool reaction or one with insufficient reactant.

The limiting case of $\lambda = 0$ corresponds to $F_N \equiv 1$, whereupon (3.2) reduces to the Liñan-Williams equation. From [1], [2] and [3] it is known that, for this case, (3.2) has a unique solution with the properties

$$(3.4) \quad u(\eta) > 0, \quad u'(\eta) > 0, \quad -\infty < \eta < \eta^*(0)$$

and asymptotic behavior

$$(3.5) \quad u(\eta) = e^\eta + \dots, \quad \eta \rightarrow -\infty,$$

$$(3.6) \quad u(\eta) = -\frac{1}{2} \log[\eta^*(0) - \eta] + \dots, \quad \eta \rightarrow \eta^*(0),$$

with the numerically determined value

$$(3.7) \quad \eta^*(0) = -0.431 \dots$$

It is the singular behavior of (3.6) which is interpreted as the achievement of ignition.

For $\lambda > 0$, the solution of (3.2) does not necessarily exhibit this singular behavior because F_N has the properties

$$(3.8) \quad F'_N(r) < 0, \quad F''_N(r) > 0, \quad 0 \leq r < \infty.$$

It is the absence of the singular behavior which has the interpretation of nonignition. Insight into the case of nonignition is gained through showing that (3.2) has a continuous solution bounded by some $\bar{M}(\lambda)$ for $-\infty < \eta < \bar{\eta}(\lambda)$. This $\bar{\eta}(\lambda)$ provides a lower bound on the time at which ignition occurs. The expressions for $\bar{\eta}(\lambda)$ and $\bar{M}(\lambda)$ are found by establishing that the integral operator in (3.2) is a contraction mapping on an appropriate space of functions.

To determine that (3.2) has a unique solution which remains bounded for all $\eta < \bar{\eta}$, consider u to be an arbitrary continuous function satisfying

$$(3.9) \quad 0 \leq u(\eta) \leq M, \quad -\infty < \eta < \bar{\eta}.$$

It then follows that

$$(3.10) \quad \begin{aligned} Tu &\equiv \int_{-\infty}^{\eta} \frac{e^{u(\xi)+\xi}}{\sqrt{\pi(\eta-\xi)}} F_N \left(\lambda \int_{-\infty}^{\xi} e^{u(\xi')+\xi'} d\xi' \right) d\xi \\ &\leq J(\eta, \lambda) e^M, \quad -\infty < \eta < \bar{\eta}, \end{aligned}$$

where

$$(3.11) \quad J(\eta, \lambda) = \int_{-\infty}^{\eta} \frac{e^{\zeta} F_N(\lambda e^{\zeta})}{\sqrt{\pi(\eta - \zeta)}} d\zeta.$$

Thus T maps the space of continuous functions satisfying (3.9) into itself whenever

$$(3.12) \quad J(\tilde{\eta}, \lambda) e^M \leq M,$$

since J is a strictly increasing function of η . To establish the contraction property of T , consider any two continuous functions u_1 and u_2 which satisfy (3.9). It then follows that

$$(3.13) \quad \sup |Tu_1 - Tu_2| \leq [J(\tilde{\eta}, \lambda) e^M + \lambda K(\tilde{\eta}, \lambda) e^{2M}] \sup |u_1 - u_2|$$

where

$$(3.14) \quad K(\eta, \lambda) = \int_{-\infty}^{\eta} \frac{e^{2\zeta} |F'_N(\lambda e^{\zeta})|}{\sqrt{\pi(\eta - \zeta)}} d\zeta.$$

In obtaining (3.13), the fact that both J and K are strictly increasing functions of η has been utilized. Hence T is a contraction operator whenever

$$(3.15) \quad J(\tilde{\eta}, \lambda) e^M + \lambda K(\tilde{\eta}, \lambda) e^{2M} < 1.$$

Thus it can be concluded that there exists a unique continuous solution of (3.2) satisfying (3.9) for any $\tilde{\eta}$ and M satisfying (3.12) and (3.15).

The largest value of $\tilde{\eta}$ satisfying (3.12) and (3.15) is found by defining $\bar{\eta}(\lambda)$ and $\bar{M}(\lambda)$ such that

$$(3.16) \quad J(\bar{\eta}, \lambda) = \bar{M} e^{-\bar{M}}, \quad \lambda K(\bar{\eta}, \lambda) = (1 - \bar{M}) e^{-2\bar{M}}.$$

For each $\lambda \geq 0$, there is a unique $\bar{\eta} \geq -1$ and $\bar{M} \leq 1$ which satisfy (3.16), and both (3.12) and (3.15) are satisfied if

$$(3.17) \quad \tilde{\eta} < \bar{\eta}(\lambda), \quad M = \bar{M}(\lambda).$$

An asymptotic analysis of (3.16) yields

$$(3.18) \quad \bar{\eta} = -1 + \frac{\lambda N}{2\sqrt{2} e} + \dots, \quad \bar{M} = 1 - \frac{\lambda N}{2\sqrt{2}} + \dots, \quad \lambda \rightarrow 0$$

and

$$(3.19) \quad \bar{\eta} = \frac{\lambda^2 \pi}{4} \bar{M}^2(\infty) e^{-2\bar{M}(\infty)} + \dots, \quad \bar{M} = \bar{M}(\infty) + \dots, \quad \lambda \rightarrow \infty,$$

where $\bar{M}(\infty) = 0.401 \dots$ uniquely satisfies the transcendental equation

$$(3.20) \quad \bar{M}(\infty) = [1 - \bar{M}(\infty)] e^{-\bar{M}(\infty)}.$$

A key result of the above analysis is that $\bar{\eta} \rightarrow \infty$ as $\lambda \rightarrow \infty$. The implication is that ignition can be indefinitely delayed by making λ sufficiently large. The fact that this is true, not just for $\lambda \rightarrow \infty$, but also for λ near unity, has been verified numerically and will be discussed later.

An asymptotic analysis of (3.2) will be carried out for two different scenarios. The first assumes that $u \rightarrow \infty$ as $\eta \rightarrow \eta^*(\lambda) < \infty$, while the second assumes that u remains bounded for all $\eta < \infty$. Each of these assumed scenarios leads to a self-consistent determination of the asymptotic behavior of u . The decision as to which scenario

applies requires an appeal to the numerical results to be given later. Those results calculate the critical value $\lambda_c(N)$ such that the first scenario applies for $\lambda < \lambda_c$ while the second applies for $\lambda > \lambda_c$.

Under the assumption that $u \rightarrow \infty$ as $\eta \rightarrow \eta^*(\lambda) < \infty$, it is convenient to define

$$(3.21) \quad \eta = \eta^* - \frac{1}{\rho}, \quad u(\eta) = v(\rho),$$

whereupon (3.2) becomes

$$(3.22) \quad v(\rho) = \rho^{1/2} e^{\eta^*} \int_0^\rho \frac{e^{v(\omega)-\omega^{-1}}}{\sqrt{\pi(\rho-\omega)} \omega^{3/2}} F_N \left(\lambda e^{\eta^*} \int_0^\omega e^{v(s)-s^{-1}} s^{-2} ds \right) d\omega.$$

Then as $\rho \rightarrow \infty$, an asymptotic solution of (3.22) is sought in the form

$$(3.23) \quad v(\rho) = \log [C_1 \rho^{1/2} + R(\rho)], \quad R(\rho) = o(\rho^{1/2}).$$

This implies that as $\rho \rightarrow \infty$

$$(3.24) \quad \frac{e^{v-\rho^{-1}}}{\rho^{3/2}} F_N \left(\lambda e^{\eta^*} \int_0^\rho e^{v(s)-s^{-1}} s^{-2} ds \right) = \frac{c_1}{\rho} F_N(\lambda e^{\eta^*} I_\infty) + o(\rho^{-1}),$$

where

$$(3.25) \quad I_\infty = \int_0^\infty e^{v(s)-s^{-1}} s^{-2} ds < \infty.$$

Then, utilizing results from [6] and [7] on the asymptotic solution of nonlinear Volterra integral equations, it follows from (3.22) that as $\rho \rightarrow \infty$,

$$(3.26) \quad v(\rho) = \frac{C_1 e^{\eta^*}}{\sqrt{\pi}} F_N(\lambda e^{\eta^*} I_\infty) \log \rho + o(\log \rho).$$

Comparison of (3.23) and (3.26) yields

$$(3.27) \quad C_1 = \sqrt{\pi} / [2 e^{\eta^*} F_N(\lambda e^{\eta^*} I_\infty)].$$

Thus, under the assumed behavior, it is found that as $\eta \rightarrow \eta^*(\lambda) < \infty$,

$$(3.28) \quad u(\eta) = -\frac{1}{2} \log(\eta^* - \eta) - \eta^* - \log [(2/\sqrt{\pi}) F_N(\lambda e^{\eta^*} I_\infty)] + o(1).$$

The actual value of $\eta^* = \eta^*(\lambda)$ must be determined numerically.

Under the second scenario, u remains bounded for all $\eta < \infty$. It is then assumed that as $\eta \rightarrow \infty$,

$$(3.29) \quad u(\eta) = d_0 \eta^\delta, \quad \delta < 1.$$

From this follows that as $\eta \rightarrow \infty$

$$(3.30) \quad e^{u+\eta} F_N \left(\lambda \int_{-\infty}^\eta e^{u(\xi)+\xi} d\xi \right) \rightarrow \frac{1}{\lambda}.$$

Then, by again utilizing the results of [6] and [7], it follows from (3.2) that as $\eta \rightarrow \infty$,

$$(3.31) \quad u(\eta) = \frac{2}{\lambda \sqrt{\pi}} \eta^{1/2} + o(\eta^{1/2}),$$

which is self-consistent with (3.29) for $\delta = \frac{1}{2}$ and $d_0 = 2/\lambda \sqrt{\pi}$.

It has now been established that there are two scenarios for the evolution of u that are compatible with (3.2). For thermal runaway, $u \rightarrow \infty$ as $\eta \rightarrow \eta^*(\lambda) < \infty$ and

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(3.28) holds; whereas in the absence of thermal runaway (3.31) holds. To know which scenario applies to a given choice of the parameter λ , a numerical analysis of (3.2) is required. The result of that analysis yields a critical value $\lambda_c = \lambda_c(N)$ such that (3.28) applies for $\lambda < \lambda_c$ and (3.31) for $\lambda > \lambda_c$.

To carry out the numerical analysis of (3.2), it is useful to have the asymptotic behavior of u as $\eta \rightarrow -\infty$. It easily follows that as $\eta \rightarrow -\infty$,

$$(3.32) \quad u(\eta) = e^\eta + \frac{1 + \lambda F'_N(0)}{\sqrt{2}} e^{2\eta} + O(e^{3\eta}).$$

It is then assumed that this expression accurately represents u on some interval $(-\infty, \eta_1)$ so that (3.2) can be put into the form

$$(3.33) \quad u(\eta) = e^{\eta_1} \operatorname{erfc} \sqrt{\eta - \eta_1} + \frac{1 + \lambda F'_N(0)}{\sqrt{2}} e^{2\eta_1} \operatorname{erfc} \sqrt{2(\eta - \eta_1)} + \int_{\eta_1}^{\eta} \frac{e^{u(\xi)+\xi}}{\sqrt{\pi(\eta-\xi)}} F(\lambda V(\xi)) d\xi, \quad \eta > \eta_1$$

where

$$(3.34) \quad V(\xi) = e^{\eta_1 + \frac{1}{2}} e^{2\eta_1} + \int_{\eta_1}^{\xi} e^{u(\xi')+\xi'} d\xi', \quad \xi > \eta_1.$$

The integrals in (3.33) and (3.34) were approximated by standard methods and the nonlinear algebraic equations resulting from the discretization were solved numerically. The scheme was begun with small values of λ , where it is expected that u will ultimately behave like (3.28). Indeed the results do indicate u becoming unboundedly large and a fit to (3.28) leads to the determination of $\eta^*(\lambda)$. Then λ is increased until this behavior ceases, and that determines $\lambda_c(N)$. These results are summarized in Tables 1 and 2.

A check on the accuracy of the algorithm is provided by the agreement between the value of $\eta^*(0)$ given in Table 2 and that of -0.431 as calculated in [1].

4. Generalized scaling of parameters. There are scalings of A and B , other than those given by (1.6) and (1.7), that lead to the same integral equation (2.33) that governs the ignition process. It is worthwhile to briefly discuss these more general scalings since they provide a broader range of parameter values under which the results derived here are applicable.

TABLE 1
Critical values of λ vs. reaction order N .

$$\lambda = b/B_0\sqrt{a}$$

$N =$	1.0	2.0	4.0
$\lambda_c =$	1.089	1.005	0.845

TABLE 2
Blow-up time t^* determined by $\eta^*(\lambda)$ vs. $\lambda < \lambda_c$ for $N = 1$.

$$t^* = t_c + (aE)^{-1}[\eta^* + \log(\sqrt{a} b/B_0)]$$

$\lambda =$	0.00	0.10	0.50	1.00	1.080	1.085
$\eta^* =$	-0.432	-0.395	-0.211	0.298	0.676	0.792

The expressions of (1.6) and (1.7) can be generalized to

$$(4.1) \quad A = E^i e^E = \left(\frac{E'}{R'\theta'_c} \right)^i \exp \left(\frac{E'}{R'\theta'_c} \right), \quad i > 0$$

and

$$(4.2) \quad B = B_0 E^{-q} = B_0 \left(\frac{R'\theta'_c}{E'} \right)^q, \quad q > 0.$$

In analogy to (1.6), here (4.1) becomes the defining relation for θ'_c . Indeed θ'_c will be essentially the same as that of (1.6), since the algebraic factor is of secondary significance.

The stretching of the independent variables in the reaction zone as given by (2.9) is replaced by

$$(4.3) \quad x = \varepsilon^m \xi, \quad t = t_c + \varepsilon^i \tau = \varepsilon^k t_0 + \varepsilon^i \tau,$$

where it is required that

$$(4.4) \quad m > 0, \quad k < i.$$

Then, the inner asymptotic expansion of θ as expressed by (2.16) becomes

$$(4.5) \quad \theta = 1 + \varepsilon [a\tau - b\xi + \phi_0(\xi, \tau)] + \varepsilon^{l+1} \phi_1(\varepsilon, \tau) + \dots,$$

where

$$(4.6) \quad l > 0,$$

and

$$(4.7) \quad a = \lim_{\varepsilon \rightarrow 0} \left[\varepsilon^{i-1} \frac{\partial \theta_I}{\partial t}(0, t_c) \right], \quad b = -\lim_{\varepsilon \rightarrow 0} \left[\varepsilon^{m-1} \frac{\partial \theta_I}{\partial x}(0, t_c) \right].$$

Here again it is required that these limits exist and that

$$(4.8) \quad a > 0, \quad b > 0.$$

For the outer asymptotic expansion of θ , the scaling of the spatial variable corresponding to (2.25) is

$$(4.9) \quad \xi = \varepsilon^{-l} X.$$

Then the outer expansion of θ as expressed by (2.26) becomes

$$(4.10) \quad \theta = \theta_I(\varepsilon^{m-l} X, t_c + \varepsilon^i \tau) + \varepsilon \Phi_0(X, \tau) + \dots$$

The derivation of the governing equations for ϕ_0 , ϕ_1 and Φ_0 together with the matching process yields the same results of § 2 provided that the scaling powers of ε are constrained to satisfy

$$(4.11) \quad 0 < i - l = \frac{3i}{2} - m = q < 1.$$

Hence the same integral equation (2.33) for f_0 is valid under any of these generalized scalings.

The results of Table 2 are then valid for a blow-up time given by

$$(4.12) \quad t^* = t_c + a^{-1} E^{-i} [\eta^* + \log(\sqrt{a} b / B_0)].$$

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