THE EFFECT OF SQUARE CORNERS ON THE IGNITION OF SOLIDS*

CARLOS VÁZQUEZ-ESPÍ† AND AMABLE LIÑÁN†

Abstract. The influence of square corners on the ignition of a solid exposed to a step in surface temperature is analyzed by means of large activation energy asymptotics. This study begins by considering the case of a semi-infinite square corner, applicable to the ignition of finite bodies with square corners when the reaction is very fast. Two spatial zones (reactive and inert) and two time stages (initial and transition) are identified. During the initial stage, the structure of the reaction zone is determined by a quasi-stationary problem of the Frank-Kamenetskii type, where the time variable plays the role of the Damköhler number. There is no solution to this problem if the time τ is larger than a certain critical value τ_0 , which is a first approximation for the ignition time. In a transition stage, for $0 < \tau_0 - \tau \ll 1$, the nonstationary effects cannot be neglected; when these are taken into account, a first correction to the ignition time is obtained. The ignition of a two-dimensional rectangular solid is also described, for which the previous analysis is partially applicable if the Damköhler number D_a is large enough. For D_a of order unity, an asymptotic analysis is given, in which the process is described in terms of a first inert heating stage and a second reacting stage ending in a thermal runaway. A numerical description is given for the second stage to determine the ignition time in terms of the Damköhler number.

Key words. combustion, ignition, thermal runaway, hot spot, activation energy asymptotics, Arrhenius kinetics

AMS subject classifications. 35C20, 35K57, 80A25

1. Introduction. When the chemical reactions occurring in combustion processes are modeled by an overall reaction, their activation energy E is large compared with the thermal energy RT . Then the reaction rate is very sensitively dependent on the temperature, so that only a small temperature increment (of the order of the Frank-Kamenetskii temperature RT^2/E) is required to increase the rate by a factor e (see [1] and [2]). The ratio of this temperature to the typical spatial temperature difference is considered as a small parameter ε , whose inverse is called the Zeldovich number in large activation energy asymptotics.

For small values of ε , we find ignition events characterized by a thermal runaway or abrupt rise in temperature occurring at a hot spot at a well-defined ignition time. During the ignition stage the reaction heat release can be neglected outside the region where the temperature differs from the maximum by an amount of the order of the Frank-Kamenetskii temperature.

It is well known that when the surface of a reacting solid is maintained at a constant temperature, equal to the initial temperature T_0 , and the Damköhler number D_a , defined as the ratio of the heat conduction time t_c to the homogeneous or adiabatic ignition time t_q , is lower than a critical value, of order unity, no ignition event in the form of a thermal runaway takes place. In this case, only a small increment in temperature is required for the conduction to the solid boundary of the heat released by the reaction. By suddenly increasing the surface temperature of a body of subcritical size to a new temperature T_s , for which the Damköhler number based on T_s is supercritical, a thermal runaway is found to occur at a well-defined

* Received by the editors March 10, 1992; accepted for publication (in revised form) December 9, 1992. This research was supported by Comisión Interministerial de Ciencia y Tecnología grant ESP-90-0271.

† Escuela Técnica Superior de Ingenieros Aeronáuticos, Universidad Politécnica de Madrid, Ciudad Universitaria, 28040 Madrid, Spain.

ignition time determined by D_a , T_0 , and T_s . See [1] and [2] for the seminal analysis of ignition processes for large activation energies and see [3] and [4] for numerical and approximate methods in ignition theory.

The techniques of large activation energy asymptotics for small values of $\varepsilon = RT_s^2/E(T_s - T_0)$ can be used to describe the changes in the structure of the ignition process that occur when the Damköhler number is reduced from very large values to the critical value (see [5] and [6]).

For very large values of D_a , the ignition time is small compared with the heat conduction time through the solid, so that the thermal wave associated with the jump in surface temperature is confined to a surface layer of thickness δ_c that is small compared with the body size a . The chemical reaction is confined to an even thinner sublayer of thickness $\varepsilon\delta_c$ adjacent to the surface, where $T_s - T \sim RT_s^2/E$. The structures of the inert conduction and reaction layers, which are one-dimensional in first approximation for $\delta_c/a \ll 1$, have been described in [7] and [8]. The analysis leads to an ignition time $t_i \sim t_q/\varepsilon^2$.

The small perturbations due to the curvature of the solid, which slightly modify the structure of the heat conduction layer, were found in [5] and [6] to shorten the ignition delay by a small amount, proportional to the product of δ_c by the local mean surface curvature. Ignition first occurs where the surface curvature is maximum. The analysis given in [8] fails, even in first approximation, if $\delta_c \sim a$; although the reaction zone structure is still one-dimensional, in first approximation, if $\varepsilon\delta_c$ is small compared with the local radius of curvature of the surface.

In this paper, we give a description of the ignition process for bodies with corners. For simplicity in the presentation and the required numerical computations, we limit the analysis to infinitely long cylindrical bodies with rectangular cross section; the analysis is also valid for rectangular straight cylinders of finite length if the bases are adiabatic. The analysis can be easily extended to describe the ignition of straight cylinders of finite length subject to a step in surface temperature.

In §2 we begin by considering the case where δ_c is small compared with a . In this case, the ignition time is determined by what happens in the corner region, which appears as semi-infinite when seen with the scale δ_c . The asymptotic analysis, given in the main text, and the numerical analysis, presented in the Appendix, lead to an ignition time $t_i \sim t_q/\varepsilon$ for the step rise in surface temperature. The ignition in a semi-infinite corner, resulting from an external heat flux, treated previously by Vorsteveld and Hermance [9] from a numerical point of view, is also amenable to an asymptotic description. The problem of ignition by step in surface temperature was treated earlier by Berman and Shevtsova [10], who attempted to explain, in terms of the roughness of the surface, the low values of the ignition time encountered in experiments. The analysis given in [10] is based on some unjustified approximations, so that their ignition time is correct only in order of magnitude.

The analysis of cylindrical bodies is considered in §3, with §3.2 devoted to the ignition for Damköhler numbers of order $D_a \sim 1/\varepsilon$, when δ_c becomes of order a . In this case, although the temperature field is determined by the body shape outside the reaction zone, the quasi-steady reaction zone structure is identical to the one described in §2.

In §3.3, we analyze the cases with Damköhler numbers of order unity for which the reaction zone, during the ignition stage, is no longer confined to the corner regions, but extends to the whole solid. We find two stages in the process: an inert heating stage of duration proportional to $\ln \varepsilon^{-1}$ and a reacting stage with a duration, depending on

the Damköhler number and body shape, that tends to infinity when D_a approaches its critical value [11]. As discussed in §3.4, a minimum value of the ignition time is found for a definite value of $D_a/D_{a,c} \sim 1$.

2. The square corner.

2.1. Formulation. Let us consider a two-dimensional reactive solid defined in polar coordinates $(\tilde{r}, \theta)$ by $\tilde{r} \geq 0$ and $0 \leq \theta \leq \pi/2$. The mathematical model, which describes the heat conduction and reaction when the surface temperature is suddenly increased from T_0 up to a constant value T_s can be formulated as

$$(2.1) \quad \rho c_s \frac{\partial T}{\partial t} = \lambda \left[\frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r} \frac{\partial T}{\partial \tilde{r}} \right) + \frac{1}{\tilde{r}^2} \frac{\partial^2 T}{\partial \theta^2} \right] + \rho q B e^{-E/RT},$$

$$(2.2) \quad T(\tilde{r}, \theta, 0) = T_0; \quad T(\tilde{r}, 0, t) = T_s, \quad T_\theta(\tilde{r}, \pi/4, t) = T_r(\infty, \theta, t) = 0 \quad \text{if } t > 0,$$

where we have considered the symmetry of the temperature profiles with respect to the line $\theta = \pi/4$. We assume that all physical properties are constant and independent of the temperature.

As a result of the increment in surface temperature, a thermal wave appears to move into the solid to raise the temperature from its initial value T_0 to the new value T_s . At the time t , the distance at which the thermal wave has entered into the solid (see Fig. 2.1), or thickness of the conduction layer, is $\delta_c \sim \sqrt{\alpha t}$, where $\alpha = \lambda/\rho c_s$ denotes the thermal diffusivity. The nonreactive solution of (2.1), (2.2), given below, shows that along the line $\theta = \pi/4$ the inert temperature distribution inside the conduction layer can be represented by the parabolic profile $T = T_s - (T_s - T_0)(\tilde{r}/\sqrt{\alpha t})^2$, while outside the temperature is still T_0 . Far from the corner, the structure of the conduction layer is one-dimensional, and the proper representation of the inert temperature is the linear profile $T = T_s - (T_s - T_0)(\tilde{x}/\sqrt{\alpha t})$, where $\tilde{x}$ is the distance normal to the surface.

The reaction zone is located near the surface, where the temperature differs from T_s by an amount of the order of the Frank-Kamenetskii temperature RT_s^2/E . As can be seen from the inert temperature profiles, the extent of the reaction region is, for a given time, much larger in the corner than away where the inert temperature decreases linearly with $\tilde{x}$. Consequently, we expect that the thermal runaway takes place near the corner at an earlier time than in any other place.

The chemical reaction produces, in the reaction zone, increments in temperature of order RT_s^2/E , whereas outside the reaction is frozen and the temperature is the inert one. In the intermediate region between the reaction zone and the conduction layer, there are no heat sources, so that the heat flux in both zones must match. Near the corner, this condition implies that $RT_s^2/E \delta_r \sim (T_s - T_0) \delta_r / \delta_c^2$, which leads to $\delta_r \sim \sqrt{\varepsilon} \delta_c$, where $\varepsilon = RT_s^2/E(T_s - T_0)$, the inverse of the Zeldovich number, is $o(1)$, according to the large activation energy limit. Similarly, we find the relation $\delta_r \sim \varepsilon \delta_c$ in the one-dimensional region. Hence, the small gradient in the corner region results in a thicker reaction zone. An order of magnitude analysis of (2.1) in the reaction zone shows that the transient term can be neglected, and then, from the balance between diffusion and chemical reaction, we obtain that the ignition time ($t_i = \delta_c^2/\alpha$) is $t_i \sim t_q/\varepsilon$ in the corner and $t_i \sim t_q/\varepsilon^2$ in the one-dimensional region, where

$$(2.3) \quad t_q = \frac{c_s R T_s^2}{q E B e^{-E/RT_s}},$$

is the homogeneous ignition time at the surface temperature.

FIG. 2.1. Schematic representation of the reaction and conduction layers in the semi-infinite square corner and inert temperature profiles.

Therefore we can conclude that, due to the geometrical effect associated with the corner, the conductive heat losses toward the interior of the solid are substantially reduced, which finally turns into a reduction of the ignition time by a factor of ϵ .

To nondimensionalize the problem, we define the dimensionless parameter $\gamma = (T_s - T_0)/T_s = O(1)$ and choose as characteristic time $t_s = t_q/\pi\epsilon$. The characteristic length is defined as $\tilde{r}_s = (\lambda t_s/\rho c_s)^{1/2}$, i.e., the depth of the conduction layer at $t = t_s$. In the nondimensional variables $\tau = t/t_s$, $r = \tilde{r}/\tilde{r}_s$, and $\varphi = (T - T_s)/(T_s - T_0)$, problem (2.1), (2.2) becomes

$$(2.4) \quad \frac{\partial \varphi}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{1}{\pi} \exp \left[\frac{1}{\epsilon} \frac{\varphi}{1 + \gamma \varphi} \right],$$

$$(2.5) \quad \varphi(r, \theta, 0) + 1 = \varphi(r, 0, \tau) = \varphi_\theta(r, \pi/4, \tau) = \varphi_r(\infty, \theta, \tau) = 0 \quad \text{if } \tau > 0.$$

From (2.4) and (2.5), it is clear that the chemical reaction is confined to a surface layer where $\varphi = O(\epsilon)$. Outside this layer, the reaction is frozen and the temperature is given by the inert distribution φ_i , i.e., the solution of (2.4), (2.5) without reaction term. Among a number of possible equivalent expressions for φ_i , the simplest one is [12, p. 171]

$$\varphi_i = -\operatorname{erf}(r \cos \theta/2\sqrt{\tau})\operatorname{erf}(r \sin \theta/2\sqrt{\tau}),$$

which, for small values of $r/\sqrt{t}$, can be written as

$$(2.6) \quad \varphi_i = -\frac{1}{\pi} \frac{r^2}{2\tau} \sin 2\theta + \frac{1}{6\pi} \left(\frac{r^2}{2\tau} \right)^2 \sin 2\theta + \dots$$

2.2. Analysis of the reaction zone. Initial stage. During the ignition period, the typical increments on temperature due to the chemical reaction are of the order of the Frank-Kamenetskii temperature RT_s^2/E . Then φ is written as $\varphi = \varphi_i + \varepsilon\psi$, to obtain the following form of (2.2):

$$\frac{\partial\psi}{\partial\tau} = \Delta\psi + \frac{1}{\pi\varepsilon} \exp\left[\frac{\psi + \varphi_i/\varepsilon}{1 + \gamma(\varepsilon\psi + \varphi_i)}\right],$$

and two zones are readily identified in the solid: an inert zone, where $\varphi_i = O(1)$ and the reaction term is exponentially small, and a reaction zone where $\varphi_i = O(\varepsilon)$. Expansion (2.6) shows that the size of the last one is given by $r^2/\tau = O(\varepsilon)$, so it is convenient to introduce the stretched similarity variable $\xi = r/\sqrt{\pi\varepsilon\tau}$ to describe the reaction zone. It follows that, in terms of this variable, problem (2.4), (2.5) can be written as

$$(2.7) \quad \pi\varepsilon \left[\tau \frac{\partial\psi}{\partial\tau} - \frac{\xi}{2} \frac{\partial\psi}{\partial\xi} \right] = \Delta\psi + \tau \exp\left[\frac{\psi + \varphi_i/\varepsilon}{1 + \gamma(\varepsilon\psi + \varphi_i)}\right],$$

$$(2.8) \quad \psi(\xi, \theta, 0) = \psi_\xi(\infty, \theta, \tau) = \psi_\theta(\xi, \pi/4, \tau) = \psi(\xi, 0, \tau) = 0,$$

where Δ is the Laplacian operator with r replaced by ξ . The solution of problem (2.7), (2.8) is sought in the form of an expansion $\psi = \psi_0 + \varepsilon\psi_1 + \varepsilon^2\psi_2 + \dots$ in the reaction zone, where ψ_i are functions of ξ , θ , and τ , and a similar expansion for the outer inert region, where the radial variable is $r/\sqrt{\pi\tau}$. In the reaction zone, where φ_i/ε can be evaluated using the expansion (2.6), under the assumption that all temporal and spatial derivatives are of order unity, we obtain the following nonlinear problem to the leading order

$$(2.9) \quad \Delta\psi_0 + \tau \exp\left[\psi_0 - \frac{1}{2}\xi^2 \sin 2\theta\right] = 0,$$

$$(2.10) \quad \psi_0(\xi, 0) = \psi_{0,\theta}(\xi, \pi/4) = \psi_{0,\xi}(\infty, \theta) = 0,$$

and the following linear one for the first correction ψ_1 :

$$(2.11) \quad \Delta\psi_1 + \tau\psi_1 \exp\left[\psi_0 - \frac{1}{2}\xi^2 \sin 2\theta\right] = \pi \left(\tau \frac{\partial\psi_0}{\partial\tau} - \frac{\xi}{2} \frac{\partial\psi_0}{\partial\xi} \right) - \tau \exp\left[\psi_0 - \frac{1}{2}\xi^2 \sin 2\theta\right] \left\{ \frac{\pi}{24} \xi^4 \sin 2\theta - \gamma \left(\psi_0 - \frac{1}{2}\xi^2 \sin 2\theta \right) \right\},$$

$$(2.12) \quad \psi_1(\xi, 0) = \psi_{1,\theta}(\xi, \pi/4) = \psi_{1,\xi}(\infty, \theta) = 0.$$

The boundary condition at $\xi = \infty$ should have been obtained from the matching conditions between the solutions corresponding to the reaction zone and the outer region ($\xi \gg 1$), where the chemical reaction is frozen; nevertheless, it is possible to justify that $\psi_\xi(\infty, \theta, \tau) = 0$ is the suitable boundary condition. To this end, first note that, for $\xi \gg 1$, (2.9) is reduced to Laplace's equation $\Delta\psi_0 = 0$, except in a boundary layer near $\theta = 0$, where $\xi^2\theta = O(1)$. As will be shown later (see the Appendix), in this layer $\psi_0 = O(\tau/\xi^2)$, so that $\psi_{0,\xi}(\infty, \theta) = 0$ and $\psi_0(\infty, \theta) = 0$ if $\theta \ll 1$. Let us consider the bounded region D defined by $1 \ll \xi_1 \leq \xi \leq \xi_2$ and

$\theta_0 \leq \theta \leq \pi/4$ with $\theta_0 = O(1/\xi_1)$ in which $\Delta\psi_0 = 0$. Then we can use the Gauss theorem to show that the total heat flux through ∂D vanishes. The heat flux also vanishes at $\theta = \pi/4$, and it is negative at $\theta = \theta_0$, because there $\psi_{0,\theta} > 0$. Hence, the heat flux is larger at $\xi = \xi_1$ than at $\xi = \xi_2$, so that $\xi \int_{\theta_0}^{\pi/4} \psi_{0,\xi}(\xi, \theta) d\theta$ is a decreasing function of ξ in D . Since ψ_0 is expected to be a smooth function, it follows that $\psi_{0,\xi} = o(1/\xi)$ for $\xi \gg 1$. Therefore, due to the fixed temperature at the wall and the geometrical effects, $\xi\psi_{0,\xi}$ tends to zero for large values of ξ , which implies not only that $\psi_{0,\xi}(\infty, \theta) = 0$, but also that $\psi_0(\infty, \theta) = 0$. The explicit form of decay of ψ_0 is obtained in [5], by solving (2.9), (2.10) for $\xi \gg 1$ and $\theta = O(1)$; the result is $\psi_0(\xi, \theta) = (4\tau/\pi)\xi^{-2} \ln \xi \sin 2\theta + o(\xi^{-2} \ln \xi)$. Note that the heat generated by the chemical reaction in the corner and in the surface reaction layer is mainly conducted to the walls and therefore does not affect the nonstationary nonreactive region. This is an important difference between the present two-dimensional problem and the one-dimensional problem analyzed in [8], where ψ at infinity was a nonzero time function and where an integral equation was obtained by matching with the outer inert region.

Since the time derivatives do not appear in (2.9), (2.10), the nondimensional time τ occurs there as a parameter, and problem (2.9), (2.10) gives the quasi-steady evolution of temperature in the reaction zone during the ignition stage. This problem is a Frank-Kamenetskii problem with τ playing the role of the Damköhler number. Therefore we expect that there exists a value of τ , say τ_0 , such that (2.9), (2.10) have solutions only if $\tau < \tau_0$. It can be proven [5] that solutions of (2.9), (2.10) exist if τ is sufficiently small and that there are no solutions if τ is sufficiently large. In the Appendix, we give some details about the numerical solution of (2.9), (2.10). The results are summarized in Fig. 2.2, which shows the maximum value of ψ_0 , $\|\psi_0\|_\infty$ as a function of τ . In this plot, we see that there are two solutions if $\tau < \tau_0 = 2.547$. The lower one is the asymptotic solution of (2.7), (2.8), since ψ_0 must satisfy the initial condition $\psi_0 = 0$. A plot of the temperature distribution at $\tau = \tau_0$ is shown in Fig. 2.3.

At $\tau = \tau_0$, the time derivative of ψ_0 is unbounded, and this constitutes the mathematical singularity characterizing the ignition. Obviously, the quasi-steady description fails for those values of $\tau < \tau_0$ such that $\partial\psi_0/\partial\tau = O(1/\varepsilon)$, so that we can distinguish two stages in the process. In the initial one, corresponding to $\tau_0 - \tau = O(1)$, the quasi-steady hypothesis is valid, and the temperature is given in first approximation by the solution of (2.9), (2.10), considered above. A more precise value of the ignition time is obtained from the analysis of a transition stage, shorter than the initial one, corresponding to small values of $\tau_0 - \tau$, where we account for unsteady effects.

2.3. Analysis of the transition stage. The kind of mathematical singularity that arises in the solution of (2.9), (2.10) at $\tau = \tau_0$ implies that the linear problem for $\psi_{0,\tau}$

$$(2.13) \quad \Delta\psi_{0,\tau} + \tau\psi_{0,\tau} \exp[\psi_0 - \tfrac{1}{2}\xi^2 \sin 2\theta] = -\exp[\psi_0 - \tfrac{1}{2}\xi^2 \sin 2\theta],$$

$$(2.14) \quad \psi_{0,\tau}(\xi, 0) = (\psi_{0,\tau})_\theta(\xi, \pi/4) = (\psi_{0,\tau})_\xi(\infty, \theta) = 0$$

has no solution at $\tau = \tau_0$. Therefore the selfadjoint problem

$$(2.15) \quad L[\phi] \equiv \Delta\phi + \tau_0\phi \exp[\varphi_0(\xi, \theta) - \tfrac{1}{2}\xi^2 \sin 2\theta] = 0,$$

$$(2.16) \quad \phi(\xi, 0) = \phi_\theta(\xi, \pi/4) = \phi_\xi(\infty, \theta) = 0,$$

FIG. 2.2. The maximum of the temperature increment due to the reaction ($\|\psi_0\|_\infty$) as a function of τ .

FIG. 2.3. Distribution of the temperature increment ψ_0 at $\tau = \tau_0$.

where $\varphi_0(\xi, \theta) = \psi_0(\xi, \theta, \tau_0)$ must possess a nontrivial eigenfunction that is not orthogonal to the term in the right-hand side of (2.13). This eigenfunction ϕ may be uniquely defined by (2.15), (2.16) with the additional conditions $\|\phi\|_\infty = 1$ and $\phi > 0$.

To find matching conditions between both the initial and transition stages, problems (2.9), (2.10) and (2.11), (2.12) must be solved when $0 < \tau_0 - \tau \ll 1$. It can be

shown [5] that ψ_0 and ψ_1 have the following asymptotic behaviour as $\tau \rightarrow \tau_0^-$:

$$(2.17) \quad \psi_0(\xi, \theta, \tau) = \varphi_0(\xi, \theta) - a_1 \sqrt{1 - \frac{\tau}{\tau_0}} \phi(\xi, \theta) + O(\tau_0 - \tau)$$

and

$$(2.18) \quad \psi_1(\xi, \theta, \tau) = -a_3 \left(1 - \frac{\tau}{\tau_0}\right)^{-1} \phi(\xi, \theta) + O(1),$$

where

$$(2.19) \quad a_1 = \left\{ 2 \frac{\int_0^\infty \int_0^{\pi/4} \phi e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta} \xi \, d\xi \, d\theta}{\int_0^\infty \int_0^{\pi/4} \phi^3 e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta} \xi \, d\xi \, d\theta} \right\}^{1/2} = 2.064 \dots$$

and

$$(2.20) \quad a_3 = \frac{\pi}{2\tau_0} \frac{\int_0^\infty \int_0^{\pi/4} \phi^2 \xi \, d\xi \, d\theta}{\int_0^\infty \int_0^{\pi/4} \phi^3 e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta} \xi \, d\xi \, d\theta} = .5344 \dots$$

From (2.17) and (2.18), it is obvious that the transition stage scale is $\tau_0 - \tau = O(\varepsilon^{2/3})$, and this leads to a new temporal variable σ and a new expansion for ψ , defined by

$$(2.21) \quad \tau = \tau_0(1 + \varepsilon^{2/3}\sigma)$$

and

$$(2.22) \quad \psi(\xi, \theta, \tau) = \varphi_0(\xi, \theta) + \varepsilon^{1/3}\varphi_1(\xi, \theta, \sigma) + \varepsilon^{2/3}\varphi_2(\xi, \theta, \sigma) + \dots$$

The equations for φ_1 and φ_2 are found to be

$$(2.23) \quad L[\varphi_1] = 0,$$

$$(2.24) \quad L[\varphi_2] = \pi \frac{\partial \varphi_1}{\partial \sigma} - \tau_0 \left(\frac{\varphi_1^2}{2} + \sigma \right) e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta},$$

to be solved with the boundary conditions (2.16). It follows that

$$(2.25) \quad \varphi_1(\xi, \theta, \sigma) = f_1(\sigma) \phi(\xi, \theta),$$

where $f_1(\sigma)$ is an arbitrary function to be determined from the solvability condition of (2.24), i.e., the orthogonality condition between the eigenfunction ϕ and the right-hand side of (2.24). This condition yields the following equation for f_1 :

$$(2.26) \quad \int_0^\infty \int_0^{\pi/4} \left[\pi \phi \frac{df_1}{d\sigma} - \tau_0 \left(\frac{1}{2} \phi^2 f_1^2 + \sigma \right) e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta} \right] \phi \xi \, d\xi \, d\theta = 0,$$

which can be written as

$$(2.27) \quad a_2 \frac{df_1}{d\sigma} = \left(\frac{f_1}{a_1} \right)^2 + \sigma,$$

where

$$(2.28) \quad a_2 = \frac{\pi}{\tau_0} \frac{\int_0^\infty \int_0^{\pi/4} \phi^2 \xi \, d\xi \, d\theta}{\int_0^\infty \int_0^{\pi/4} \phi e^{\varphi_0 - \frac{1}{2}\xi^2 \sin 2\theta} \xi \, d\xi \, d\theta} = .5018 \dots$$

The initial condition for (2.27) is obtained from the matching condition with (2.17) to be

$$(2.29) \quad f_1 \sim -a_1 \sqrt{-\sigma} \quad \text{as } \sigma \rightarrow -\infty.$$

The Riccati equation (2.27), which appears in some related problems [13, p. 75], [14], can be reduced to the Airy equation by means of a standard transformation, and the solution satisfying the initial condition (2.29) is

$$(2.30) \quad f_1 = a_1^{4/3} a_2^{1/3} \frac{1}{A_i(-s)} \frac{dA_i(-s)}{d(-s)},$$

where A_i is the Airy function and $s = \sigma/(a_1 a_2)^{2/3}$. The function $A_i(-s)$ only vanishes if $s > 0$, with the first root at $s = 2.3381 \dots$. Therefore the temperature $\varphi_1 = f_1(\sigma) \phi(\xi, \theta)$ diverges at $\sigma_0 = 2.3381(a_1 a_2)^{2/3}$; then the ignition time, as determined from the transition stage analysis, is given by

$$(2.31) \quad \tau_i = \tau_0(1 + 2.3381(\varepsilon a_1 a_2)^{2/3}),$$

or in dimensional variables (the chemical time t_q is defined in (2.3))

$$(2.32) \quad \frac{t_i}{t_q} = \frac{1}{\pi \varepsilon} (2.547 + 6.096 \varepsilon^{2/3}).$$

The analogous relation for the one-dimensional case [8] is $t_i/t_q = (1/2\pi\varepsilon^2)(1 - 2\varepsilon \ln \varepsilon + O(\varepsilon))$. Hence the square corner reduces the ignition time by a factor of ε . Note that, while the temperature distribution in the initial stage has a singularity in the time derivative, the transition distribution has singularities in both the function and the derivative.

These results break down when f_1 grows up to values of order $\varepsilon^{-1/3}$. In the subsequent evolution, from the formation of a hot spot to the development of a flame, large departures from the inert temperature take place; so it cannot be described using ignition methods. An analysis similar to [15] will probably be suitable. As has been pointed out by one of the referees, the flame generated at the hot spot in the corner will first propagate along the higher temperature layer adjacent to the wall before reaching the interior of the solid.

3. The ignition of a cylindrical solid of rectangular cross section.

3.1. Formulation. In the previous section, we analyzed the ignition process in a semi-infinite square corner, and now we describe the ignition of a cylindrical solid of rectangular cross section. The length of the body is infinite, or finite with adiabatic end cross sections, so that the temperature field is two-dimensional. Most of the ideas used in the remainder of the paper are similar to those in [6], where more general cases are considered; some details are omitted here for brevity. As in [6], we find three different regimes corresponding to three different ranges of Damköhler number values. The results of §2 are applied directly in the first regime and partially in

the second regime, while, in the third regime, we must carry out some numerical calculations.

Let us consider a reactive body of rectangular shape with dimensions $2a$ and $2b$ ($b \geq a$). Using the assumptions of §2.1 for the physical properties, chemical reaction, and how to produce ignition, the equation and boundary and initial conditions describing the evolution of the temperature in the domain $\Omega = [0, 2a] \times [0, 2b]$ are

$$(3.1) \quad \rho c_s \frac{\partial T}{\partial t} = \lambda \Delta T + \rho q B e^{-E/RT},$$

$$(3.2) \quad T(\tilde{x}, \tilde{y}, 0)|_{\Omega} = T_0, \quad T(\tilde{x}, \tilde{y}, t)|_{\partial\Omega} = T_s \quad (t > 0).$$

Two characteristic times are involved in this equation: the conduction time $t_c = \rho c_s a^2 / \lambda$ and the homogeneous ignition time $t_q = c_s R T_s^2 / q E B e^{-E/RT_s}$; the ratio defines the Damköhler number $D_a = \rho q B E a^2 / \lambda R T_s^2 e^{E/RT_s}$. To nondimensionalize the above problem, we introduce the parameters γ and ε , defined in §2, and a new geometrical parameter $l = b/a \geq 1$ measuring the slenderness of the cross section. Using the dimensionless variables $\varphi = (T - T_s)/(T_s - T_0)$, $\tau = t/t_c$, and $(x, y) = (\tilde{x}, \tilde{y})/a$, problem (3.1), (3.2) can be written in the form

$$(3.3) \quad \frac{\partial \varphi}{\partial \tau} = \Delta \varphi + \varepsilon D_a \exp \left[\frac{1}{\varepsilon} \frac{\varphi}{1 + \gamma \varphi} \right],$$

$$(3.4) \quad \varphi(x, y, 0) + 1 = \varphi(0, y, \tau) = \varphi(x, 0, \tau) = \varphi_x(1, y, \tau) = \varphi_y(x, l, \tau) = 0$$

in the domain $[0, 1] \times [0, l]$. The problem of finding slowly burning, stationary solutions of (3.3) with the boundary condition (3.4) in the limit $\varepsilon \rightarrow 0$ with bounded values of φ/ε leads to the Frank-Kamenetskii problem. Then the time derivative in (3.3) is omitted and γ is replaced by zero. It is well known that solutions of this problem exist only for subcritical values $D_a < D_{a,c}$ of the Damköhler number. For supercritical values, we encounter a thermal runaway at an ignition time that becomes infinite when $D_a \rightarrow D_{a,c}$.

If the heat conduction time t_c is large compared with the ignition time of the corner analysis of §2, $O(t_q/\varepsilon)$, then t_i is given by (2.32). However, the ignition time is decreased by a factor of order unity becoming of order t_c , when $D_a = t_c/t_q$ is lowered to values of order $1/\varepsilon$; in this case, the thermal wave during the ignition stage has reached the core of the cylinder, and the inert temperature close to the corner is no longer given by (2.6).

3.2. Analysis of the case where $D_a \gg 1$. Thus, when $D_a \sim 1/\varepsilon$ or larger, the chemical effects are confined to a thin surface layer, and therefore we can distinguish two zones inside the solid: a reactive-diffusive reaction zone located near the surface and a nonsteady inert conduction zone (see Fig. 3.1). The matching between both zones allows us to obtain the order of magnitude of the ignition time $t_i = O(t_c/\varepsilon D_a)$. If $\varepsilon D_a \gg 1$, the ignition delay is much shorter than the conduction time through the solid, so that, when ignition occurs, the thermal wave is confined to a thin layer, and the solid appears as semi-infinite; therefore we expect the results of §2 to be directly applicable. The reaction zone is still confined to a surface layer if $\varepsilon D_a \sim 1$, but the thermal wave reaches the central region of the solid before the ignition runaway. As a consequence, the inert-temperature gradient at the surface is different from that in the semi-infinite solid case, and this changes the ignition time. The cases where $\varepsilon D_a \sim 1$ and $\varepsilon D_a \gg 1$ are considered simultaneously by analyzing the distinguished limit $\varepsilon D_a \sim 1$.

FIG. 3.1. Schematic representation of the reaction and conduction layers in the cylindrical solid of rectangular cross section in the cases where $D_a \gg 1/\epsilon$ and $D_a \sim 1/\epsilon$.

For the analysis of the reaction zone, we use the difference between the temperature φ and its inert value φ_i as dependent variable. For small values of x and y , i.e., near corner, φ_i can be represented as

$$(3.5) \quad \varphi_i = -xyA(\tau, l) + o(xy),$$

where $A(\tau, l)$ is a strictly positive decreasing function of time. This function can be calculated by means of infinite series with two equivalent expressions: one converges very quickly for $\tau \ll 1$, and the other for $\tau = O(1)$ [12, pp. 171–173]. The leading term of the first of these series provides the following approximations for $A(\tau, l)$ when $\tau \ll 1$:

$$(3.6) \quad A(\tau, l) \simeq \frac{1}{\pi\tau},$$

while, for $\tau = O(1)$, we use the series

$$(3.7) \quad A(\tau, l) = \frac{4}{l} \sum_{m,n=0}^{\infty} \exp \left\{ -\frac{\pi^2}{4} \left[(2n+1)^2 + \left(\frac{2m+1}{l} \right)^2 \right] \tau \right\} \quad \text{for } l = O(1),$$

$$A(\tau, l) = \frac{2}{\sqrt{\pi\tau}} \sum_{n=0}^{\infty} \exp \left\{ -\frac{\pi^2}{4} (2n+1)^2 \tau \right\} \quad \text{for } l \gg 1.$$

Figure 3.2 shows the function $A(\tau, l)$ for several values of l and its leading term representations for $l = 1.5$.

During the ignition period, the increments in the temperature above its inert value are of the order of the Frank-Kamenetskii temperature ϵ ; so, we use $\psi = (\varphi - \varphi_i)/\epsilon$ as variable. The form of the inert temperature (3.5) shows the convenience of using

$$(3.8) \quad (\xi, \eta) = \sqrt{\frac{A(\tau, l)}{\epsilon}}(x, y)$$

as space variables for the reaction zone. Problem (3.3), (3.4) becomes

$$(3.9) \quad \epsilon \left[\frac{1}{A} \frac{\partial \psi}{\partial \tau} + \frac{1}{2A^2} \frac{\partial A}{\partial \tau} \left(\xi \frac{\partial \psi}{\partial \xi} + \eta \frac{\partial \psi}{\partial \eta} \right) \right] = \Delta \psi + \frac{\epsilon D_a}{A} \exp \left[\frac{\psi - \xi \eta + O(\epsilon)}{1 + \gamma \epsilon (\psi - \xi \eta) + o(\epsilon)} \right],$$

FIG. 3.2. The function $A(\tau, l)$ characterizing the inert temperature in the corner region, as a function of τ for $l = 1, 1.5, 2, \infty$.

$$(3.10) \quad \psi(\xi, \eta, 0) = \psi(0, \eta, \tau) = \psi(\xi, 0, \tau) = \psi_\xi(\infty, \eta, \tau) = \psi_\eta(\xi, \infty, \tau) = 0.$$

When, for values of $\varepsilon D_a/A$ of order unity, we look for the solution of this problem as an expansion $\psi = \psi_0 + \varepsilon\psi_1 + \dots$, we encounter the following problem for ψ_0 :

$$(3.11) \quad \Delta\psi_0 + \frac{\varepsilon D_a}{A} \exp[\psi_0 - \xi\eta] = 0,$$

$$(3.12) \quad \psi_0(\xi, 0) = \psi_0(0, \eta) = \psi_{0,\xi}(\infty, \eta) = \psi_{0,\eta}(\xi, \infty) = 0,$$

identical to (2.9), (2.10) if $\varepsilon D_a/A$ is replaced by τ . The results of §2 show that solutions of problem (3.11), (3.12) exist only if $\varepsilon D_a/A < 2.547$; therefore the ignition time τ_0 is determined in first approximation by the relation

$$(3.13) \quad 2.547 A(\tau_0, l) = \varepsilon D_a.$$

Hence, $A(\tau_0, l) \gg 1$ if $\varepsilon D_a \gg 1$, and then τ_0 is given, according to (3.6), by $\tau_0 = 2.547/\pi\varepsilon D_a \ll 1$, the result obtained in §2. For $\varepsilon D_a \sim 1$ ($D_a \sim 1/\varepsilon \gg 1$), the ignition time τ_0 , if moderately large compared with 1, is given by

$$(3.14) \quad \begin{aligned} \tau_0 &= \frac{4}{\pi^2(1+1/l^2)} \ln\left(2.547 \frac{4}{\varepsilon l D_a}\right) \quad \text{for } l = O(1), \\ \frac{\pi^2}{2} \tau_0 + \ln \tau_0 &= 2 \ln \frac{5.094}{\sqrt{\pi\varepsilon D_a}} \quad \text{for } l \gg 1. \end{aligned}$$

The initial stage ends when $0 < \tau_0 - \tau \ll 1$ (i.e., when the quasi-stationary description fails), and it is followed by a transition stage in which the unsteady effects

must be retained. The analysis of this short stage is analogous to that of §2, with the coefficients a_1 , a_2 , and a_3 being replaced by the generalized coefficients b_1 , b_2 , and b_3 , defined by

$$(3.15) \quad \begin{aligned} b_1 &= a_1(-\tau_0 \dot{A}_0/A_0)^{1/2}, \\ b_2 &= a_2/(-\pi\tau_0^2 \dot{A}_0), \\ b_3 &= a_3/\pi\tau_0 A_0, \end{aligned}$$

where $A_0 = A(\tau_0, l)$ and $\dot{A}_0 = \partial A(\tau_0, l)/\partial \tau$. As in §2, we obtain the following corrected value for the ignition time:

$$(3.16) \quad \tau_i = \tau_0(1 + 2.3381(\varepsilon b_1 b_2)^{2/3})$$

if terms of order ε are omitted. Note that $b_i = a_i$ for $\varepsilon D_a \gg 1$, recovering the results of §2. In Fig. 3.3, the product $b_1 b_2$ is shown as a function of εD_a . The analysis fails for small values of εD_a , i.e., $D_a = O(1)$, when $b_1 b_2$ becomes large, and the transition stage is no longer short compared with the initial one. The ignition time as a function of εD_a is plotted in Fig. 3.4 ($\varepsilon = 0, 1/25$ and $l = 1, 1.5, 2$). The values of $b_1 b_2$ and τ_i for $l = \infty$ cannot be distinguished in Figs. 3.2 and 3.4 from those of $l = 2$.

FIG. 3.3. The coefficient $b_1 b_2$ determining the corrected value for the ignition time as a function of εD_a for $l = 1, 1.5, 2$.

3.3. Analysis of the case where $D_a = O(1)$. We see from (3.3) that the reaction term only leads to changes in φ of order ε after the growth of φ from its initial value (-1) to a value $\varphi = O(\varepsilon)$. During this heating stage, the temperature is determined by the inert problem (i.e., (3.3), (3.4) without reaction term), easily solved by separation of variables. We must wait until τ is moderately large compared with unity for $(-\varphi)$ to decay to a value of order ε and thus initiate the reacting stage.

FIG. 3.4. The ignition time τ_i corresponding to $\epsilon D_a \gg 1$ as a function of ϵD_a for $\epsilon = 0, 1/25$ and $l = 1, 1.5, 2$.

At this time, the inert temperature can be represented by the slowest decaying mode $\varphi_i = -(16/\pi^2) \exp[-\pi^2(1 + 1/l^2)\tau/4] \sin(\pi x/2) \sin(\pi y/2l)$. If we want $\varphi_i = O(\epsilon)$, then $\tau \sim \tau_\epsilon$, where τ_ϵ is defined by

$$(3.17) \quad \tau_\epsilon = \frac{4 \ln(1/\epsilon)}{\pi^2(1 + 1/l^2)}.$$

To describe the reaction stage that defines the ignition time, we use the variables $\hat{\tau} = \tau - \tau_\epsilon$ and $\psi = \varphi/\epsilon$. The initial condition (3.4) can be replaced by the matching condition for $\hat{\tau} \rightarrow -\infty$ with the slowest decaying mode of φ_i . To the lowest order, the resulting problem is

$$(3.18) \quad \frac{\partial \psi}{\partial \hat{\tau}} = \Delta \psi + D_a e^\psi,$$

$$(3.19) \quad \psi(0, y, \hat{\tau}) = \psi(x, 0, \hat{\tau}) = \psi_x(1, y, \hat{\tau}) = \psi_y(x, l, \hat{\tau}) = 0,$$

$$(3.20) \quad \hat{\tau} \rightarrow -\infty : \psi = -\frac{16}{\pi^2} \exp\left[-\frac{\pi^2}{4}(1 + 1/l^2)\hat{\tau}\right] \sin \frac{\pi}{2} x \sin \frac{\pi}{2} \frac{y}{l}.$$

This problem was solved numerically, for given values of D_a and l , by a Newton-Kantorovich method, with a spatial discretization via a finite volume method. The Crank-Nicholson method was used with a variable time stepsize to obtain rapidly convergent solutions, even at times close to the ignition time when $\partial \psi / \partial \hat{\tau}$ becomes large.

For fixed l and D_a larger than some critical value $D_{a,c}(l)$, the solution of this problem shows blowup at $\hat{\tau}_i = \hat{\tau}_i(D_a, l)$, while, for smaller values of D_a , the solution remains bounded for all $\hat{\tau}$. As has been shown by Dold [16], the temperature increment

at the hot-spot kernel during the final stage of the thermal runaway has a universal structure, which is independent of the initial conditions. In particular, the maximum value of the solution of (3.18)–(3.20) has the behaviour $-\ln(D_a(\hat{\tau}_i - \hat{\tau}))$ for $\hat{\tau}_i - \hat{\tau} \ll 1$, which we used to accurately determine the value of $\hat{\tau}_i$. Figure 3.5 shows $\hat{\tau}_i$ in terms of D_a for $l = 1, 1.5$, and 2 . The corresponding critical Damköhler numbers $D_{a,c}$, computed from the stationary problem associated with (3.18)–(3.19), are 1.702, 1.230, and 1.066, respectively. Note that these values are the leading order term of an expansion of $D_{a,c}$ in powers of ε [17]. The asymptotic solution of (3.18)–(3.20) for $D_a \gg 1$ leads to the ignition time

$$(3.21) \quad \hat{\tau}_i(D_a \gg 1) \simeq \frac{4}{\pi^2(1 + 1/l^2)} \ln\left(2.547 \frac{4}{lD_a}\right),$$

in agreement with (3.14).

FIG. 3.5. The duration of the reaction stage $\hat{\tau}_i$ as a function of D_a for $l = 1, 1.5, 2$.

In Fig. 3.6, we show the distributions of ψ at $\hat{\tau}_i$ for $l = 1$ and three values of D_a . Note the transition as D_a grows from the self-ignition mode ($D_a = 4$ in Fig. 3.6), where the temperature rises at every point of the solid ending with a hot spot at the center, to the forced ignition regime ($D_a = 60$ in Fig. 3.6), where the point of maximum temperature is located near the corner, while we still have the inert temperature at the center. For moderately large values of D_a ($D_a = 15$ in Fig. 3.6), the hot spot is not placed at the center, although the thermal wave produces a significant increment of the temperature of the whole solid before the ignition runaway.

For $l = \infty$, the resulting problem is very similar to (3.18)–(3.20). The initial condition (3.19) must be replaced by $\psi = -(4/\pi) \operatorname{erf}(y/2\sqrt{\tau_\varepsilon + \hat{\tau}}) e^{-\pi^2 \hat{\tau}/4} \sin(\pi x/2)$ for $0 < \tau_\varepsilon + \hat{\tau} \ll 1$. Due to the form of the inert distribution, it is not possible to remove the parameter ε from the initial condition; so this problem must be solved for several values of ε . Figure 3.7 shows τ_i as a function of D_a for $\varepsilon = 1/50, 1/25$, and $1/10$.

FIG. 3.6. Distribution of the temperature ψ at the ignition time for the square cross section ($l = 1$) and $D_a = 4, 15, 60$. (Only a quarter of the section is shown for $D_a = 15$ and 60 .)

The analysis of this section fails for large values of D_a , when the ignition time becomes smaller than the conduction time and the splitting into two stages (inert heating and reacting) is not valid. However, in this case, we may use the analysis of the previous section.

3.4. Minimum ignition time. It is convenient to refer the ignition time to the homogeneous ignition time t_q , which is independent of the solid size. To calculate the ratio t_i/t_q , we must multiply the values of the ignition time τ_i and $\tau_\varepsilon + \hat{\tau}_i$, obtained

FIG. 3.7. The ignition time, τ_i , corresponding to semi-infinite slabs (solid lines) and infinite slabs (dashed lines) as a function of D_a for $\epsilon = 1/50, 1/25, 1/10$.

in §§3.2 and 3.3, by D_a . In this way, the curves of Fig. 3.8 are obtained for $\epsilon = 1/25$ and the extreme values $l = 1$ and $l = \infty$, as well as for the infinite slab. Note the differences, for large Damköhler numbers, in the ignition times of the slab and the semi-infinite slab ($l = \infty$), which are due to the effect of the square corners. For other values of l and ϵ , the corresponding curves are qualitatively similar. As we also find for more general shapes, a minimum value of t_i/t_q is found for given l and ϵ at a value of the Damköhler number slightly larger than the critical one. For each value of ϵ , we obtain, from the definition of $\hat{\tau}$, the following relations that determine the values $t_{i,m}$ and $D_{a,m}$ of t_i and D_a corresponding to the minimum ignition time:

$$(3.22) \quad \frac{4}{\pi^2} \frac{\ln(1/\epsilon)}{1 + 1/l^2} = -\hat{\tau}(D_{a,m}) - D_{a,m} \frac{\partial \hat{\tau}(D_{a,m})}{\partial D_a}$$

and

$$(3.23) \quad \frac{t_{i,m}}{t_q} = -D_{a,m}^2 \frac{\partial \hat{\tau}(D_{a,m})}{\partial D_a}.$$

The results are represented in Fig. 3.9, showing that the ratios $t_{i,m}/t_q$ and $D_{a,m}/D_{a,c}$ are nearly independent from the slenderness l . Note that the minimum ignition time is slightly larger for the infinite slab than for the semi-infinite slab. For this, the numerical results show that the hot spot moves from near the corner for large values of D_a to a point located on the axis of symmetry at a distance from the edge of about $3a$, when D_a decreases to $D_{a,m}$.

The numerical results given in Fig. 3.9 for the minimum ignition time for infinite slabs can be used to calculate the ignition time of wedges of angle $\alpha \ll 1$. For these, the radial conduction can be neglected; the behaviour of the wedge at each radial

FIG. 3.8. The ignition time t_i/t_q for the square cross section ($l = 1$), the semi-infinite slab ($l = \infty$), and the infinite slab, as a function of D_a for $\epsilon = 1/25$.

FIG. 3.9. Values of D_a and t_i corresponding to the minimum ignition time as a function of ϵ , for different finite rectangular cross sections ($l = 1, 1.5, 2$), semi-infinite slab ($l = \infty$), and infinite slab.

station is nearly identical to that of an infinite slab with a Damköhler number that increases with the square of the distance to the vertex. A hot spot will first appear at a distance from the vertex where $D_a = D_{a,m}(\varepsilon)$ at a time $t_i = t_{i,m}$, which is also a function only of ε plotted in Fig. 3.9.

4. Results and conclusions. The ignition of a reactive two-dimensional rectangular solid exposed to a step in surface temperature has been analyzed in the limit of large activation energies. We have obtained the value of the ignition time for all values of the Damköhler number above the critical.

If $D_a \gg 1/\varepsilon$, the ignition delay is very small compared with the conduction time, and the thermal runaway characterizing the ignition takes place near the corners, where the gradients of the inert temperature are small. For the description of the ignition process for these large values of D_a , the solid can be modeled by a semi-infinite square corner. The analysis given in §2 shows the existence of two stages in the ignition process. During the first, longer, stage the structure of the reaction zone is quasi-stationary; the temperature increment due to the chemical reaction is described by a nonlinear equation, in which the time appears as the only parameter. Solutions of this equation exist only for values of the time smaller than a critical value, which determines the ignition time in first approximation. The turning point singularity in the solution is removed in the analysis of a second transition stage, where the effect of the nonstationary term is included to obtain a correction to the ignition time. When the ignition time for the square corner, given by $t_i = 2.547t_q/\pi\varepsilon$ in first approximation, is compared with that of a semi-infinite planar body $t_i = t_q/2\pi\varepsilon^2$, we find a reduction of order ε in the ignition time. The same procedure was used in [5] to calculate the ignition times for corners with angles α different from $\pi/2$ or π resulting in $t_i/t_q = c(\alpha)/\varepsilon^{2\alpha/\pi}$, where $c(\alpha)$ is an order unity function of α plotted in Fig. 4.1. For decreasing values of α , the solid becomes less and less supercritical, so that the quasi-stationary description, similar to that of §2, fails even in first approximation; for the determination of the ignition time of these small angle wedges, see the end of §3.4. The formulation of the analysis of the ignition process for three-dimensional corners is straightforward, but the numerical calculations are considerably more difficult, except in some symmetrical cases as cones [5].

In the distinguished limit $D_a = O(1/\varepsilon)$, the reaction, during the ignition transient, is confined to a small region near the corner, but the ignition time is of the same order as the conduction time. As a consequence, the thermal wave reaches the central region during the ignition process, and the inert temperature distribution must include the effect of the finite size of the solid. The structure of the reaction zone is identical to that of §2, determined by a function $A(\tau, l)$, which characterizes the inert temperature near the corners. The results show that the ignition time is, as we would expect, an increasing function of D_a and of the slenderness l .

When $D_a = O(1)$, it is not possible to distinguish the two spatial zones, reactive and inert, which appeared if $D_a \gg 1$. Instead, we now find two temporal stages: a first inert heating stage of duration defined by (3.17) and a slightly shorter reaction stage that ends in a thermal runaway. In the reaction stage, the temperature is given by the solution of a nonlinear parabolic problem containing D_a and l as parameters. This problem has been solved numerically for different values D_a and l to obtain the time $\hat{\tau}_i$, which, when added to the time τ_ε corresponding to the first stage, gives the ignition time $\tau_\varepsilon + \hat{\tau}_i$. We find that, for given values of ε and l , there is a minimum value of the ignition time $t_{i,m}$, corresponding to a value $D_{a,m}$ of the Damköhler number. The ratios $D_{a,m}/D_{a,c}$ and $t_{i,m}/t_q$, shown in Fig. 3.9, are functions of ε weakly dependent

FIG. 4.1. The reduced ignition time $\varepsilon^{2\alpha/\pi} t_i / t_q$ for wedges with angles α such that $\pi/4 < \alpha < \pi$ as a function of α .

on l . We also show in Fig. 3.9 the values of these ratios for one-dimensional slabs and for semi-infinite slabs.

It should be noted that the critical value of the Damköhler number, evaluated here by numerical integration for infinitely long cylindrical bodies of rectangular cross section, decreases from the value $D_{a,c} = 1.702$ for $l = 1$ to the value $D_{a,c} = 0.879$ for $l = \infty$, corresponding to slabs. We may expect negligible effects on $D_{a,c}$ of the nonadiabatic end sections in long cylinders of finite length (see [18] for a rigorous analysis). The end sections will, however, affect the ignition time for large values of D_a . Note, for example, the strong reduction in the ignition time, due to the effect of the square corners in the case where $l \rightarrow \infty$, as compared with the infinite slab without side edges. An order of magnitude analysis [5] indicates that the ignition time for large values of D_a is of order $t_q / \varepsilon^{2/3}$ for bodies with three-dimensional square corners.

The analysis given here can be used to describe the ignition of thin, coin-shaped plates (bounded by a smooth, straight, cylindrical surface) if the ratio of their thickness $2a$ to the characteristic dimension L of the surface of the plates is small. In this case, the critical Damköhler number is that of slabs of thickness $2a$, determined by heat conduction normal to the plate. For large Damköhler numbers, ignition will occur first close to the edges in an edge region of transverse size $2a$; the solid appears as a semi-infinite slab when seen with the scale of this region, and the ignition time is shown in Fig. 3.7 as a function of the Damköhler number.

In this work, we have not considered the effect of the reactant consumption under the assumption that the heat of reaction q is very large. In fact, the present formulation of the problem corresponds to the cases for which the parameters $c_s(T_s - T_0)/q$, for $D_a \gg 1$ and $c_s R T_s^2 / q E$ for $D_a \sim 1$ that measure the effect

of reactant consumption are small compared with unity. The analysis of the ignition process for finite values of these parameters will be considered elsewhere.

Appendix. Numerical solution of problem (2.9), (2.10). In §2 we found that the problem to be solved to determine the first approximation of the temperature increment was

$$(A.1) \quad \Delta\psi + \tau \exp\left[\psi - \frac{1}{2}\xi^2 \sin 2\theta\right] = 0,$$

$$(A.2) \quad \psi(\xi, 0) = \psi_\theta(\xi, \pi/4) = \psi_\xi(\infty, \theta) = 0,$$

where for simplicity we have omitted the subindex. The ignition time appears as the maximum value of τ for which (A.1), (A.2) has solution.

This problem must be solved numerically. The unboundedness of the domain introduces difficulties that cannot be overcome easily. To properly treat the boundary condition $\psi_\xi(\infty, \theta) = 0$, it must be transferred to a finite position, say $\xi = \xi_\infty$. Obviously, the boundary condition at a finite value ξ_∞ of ξ cannot be replaced by $\psi_\xi(\xi_\infty, \theta) = 0$, since it would be equivalent to consider that the restricted domain of the solid is adiabatically isolated in the radial direction, and therefore we would prevent the heat flux from reaching the outer wider zones. In the corner case, there are heat conduction losses to the walls not existing in the one-dimensional case so that $\xi\psi_\xi$, or the total radial heat flux, decreases, although slowly, with $\xi \rightarrow \infty$. In fact, as shown in [5], the behaviour of ψ for $\xi \gg 1$ and $\theta = O(1)$ is given by $\psi = (4\tau/\pi)\xi^{-2} \ln \xi \sin 2\theta + o(\xi^{-2} \ln \xi)$.

The procedure that we use to obtain the new boundary condition at ξ_∞ takes advantage of the special form that problem (A.1), (A.2) adopts for $\xi \gg 1$. It can be outlined as follows:

(i) We choose a value of ξ_∞ large enough so that the chemical reaction is frozen; hence (A.1) reduces to the Laplace equation. This is true, except in a surface boundary layer where $\theta\xi^2 \sim 1$. As we show later, there are stronger gradients of temperature in this layer in the rest of the curve $\xi = \xi_\infty$;

(ii) We then solve problem (A.1), (A.2), plus the additional condition $\psi(\xi_\infty, \theta) = g(\theta)$ in the unbounded domain $]\xi_\infty, \infty[\times]0, \pi/4[$, where g is an unknown function. Therefore the outer problem can be formulated as solving (A.1) with conditions (A.2) replaced by

$$(A.3) \quad \psi(\xi_\infty, \theta) - g(\theta) = \psi(\xi, 0) = \psi_\theta(\xi, \pi/4) = \psi_\xi(\infty, 0) = 0.$$

(iii) From the solution of this problem, we can compute $\psi_\xi(\xi_\infty, \theta) = f(\theta)$. Since the function f depends on the function g , the condition $\psi_\xi(\xi_\infty, \theta) - f(\theta) = 0$ can be seen as the relation to be satisfied by both $\psi(\xi_\infty, \theta)$ and $\psi_\xi(\xi_\infty, \theta)$ to ensure that $\psi_\xi(\infty, \theta) = 0$; we write this relation formally as $B[\psi(\xi_\infty, \theta), \psi_\xi(\xi_\infty, \theta)] = 0$. This relation, which is analogous to the integral equation found in the one-dimensional problem when matching both the reaction and inert zones, is the new mixed boundary condition to be imposed on the inner problem corresponding to the domain $]0, \xi_\infty[\times]0, \pi/4[$.

We see below how problem (A.1), (A.3) leads to an analytical expression for the heat flux $f(\theta)$ in terms of $g(\theta)$. Then we can reformulate problem (A.1), with (A.2) solved as (A.1), in the bounded domain $]0, \xi_\infty[\times]0, \pi/4[$, with the boundary conditions

$$(A.4) \quad \psi(\xi, 0) = \psi_\theta(\xi, \pi/4) = B[\psi(\xi_\infty, \theta), \psi_\xi(\xi_\infty, \theta)] = 0.$$

Solution of the outer problem. Problem (A.1), (A.2), when using the variable $\eta = \xi/\xi_\infty = O(1)$, takes the form

$$(A.5) \quad \Delta\psi + \tau\xi_\infty^2 \exp\left[\psi - \frac{1}{2}\xi_\infty^2\eta^2 \sin 2\theta\right] = 0,$$

$$(A.6) \quad \psi(\eta, 0) = \psi_\theta(\eta, \pi/4) = \psi(1, \theta) - g(\theta) = \psi_\eta(\infty, \theta) = 0.$$

The nonlinear term in (A.5) becomes exponentially small for $\xi_\infty \gg 1$, except if $\theta \sim 1/\xi_\infty^2 \ll 1$. Therefore we can distinguish two different zones in the outer region: a boundary layer located around $\theta = 0$, in which the reaction term must be retained, and a conduction zone where $\theta = O(1)$ and (A.5) is reduced to the Laplace equation.

The suitable variables to analyze the boundary layer are $x = \xi_\infty^2\theta$ and $V(\eta, x) = \xi_\infty^2\psi$, given to leading order the problem

$$(A.7) \quad \frac{1}{\eta^2} \frac{\partial^2 V}{\partial x^2} + \tau e^{-\eta^2 x} = 0; \quad V(\eta, 0) = 0,$$

whose solution is

$$(A.8) \quad V(\eta, x) = A\eta^2 x + \frac{\tau}{\eta^2} (1 - e^{-\eta^2 x}).$$

Matching with the conduction zone yields $A = 0$, so the temperature at $\theta = 0$ as seen from the conduction zone is $V(\eta, x \rightarrow \infty)/\xi_\infty^2 = \tau/\xi_\infty^2$. Hence, the effect of the boundary layer is to produce a jump in the surface temperature, and the boundary condition to be applied at $\theta = 0$ to the Laplace equation must be modified. In the conduction zone, we write $\psi = U(\eta, \theta)/\xi_\infty^2$, with $U(\eta, \theta)$ given to the leading order by

$$(A.9) \quad \Delta U = 0,$$

$$(A.10) \quad U(\eta, 0) - \frac{\tau}{\eta^2} = U(1, \theta) - \xi_\infty^2 g(\theta) = U_\theta(\eta, \pi/4) = U_\eta(\infty, \theta) = 0.$$

We can write $U = F_1 + F_2 + \tau/\eta^2$, where F_1 satisfies a Laplace problem with nonhomogeneous boundary conditions and where F_2 is a Poisson problem with homogeneous boundary conditions. The first can be solved easily by using separation of variables, yielding

$$(A.11) \quad F_{1,\eta}(1, \theta) = -\sqrt{\frac{8}{\pi}} \sum_{n=1}^{\infty} \lambda_n a_n(\tau) \sin \lambda_n \theta,$$

where

$$(A.12) \quad \lambda_n = 2(2n-1) \quad \text{and} \quad a_n(\tau) = \sqrt{\frac{8}{\pi}} \int_0^{\pi/4} (\xi_\infty^2 g(\theta) - \tau) \sin \lambda_n \theta \, d\theta.$$

The second can be solved using the proper Green's function technique to yield

$$(A.13) \quad F_{2,\eta}(1, \theta) = \frac{2\tau}{\pi} (\sin 2\theta \ln(2 \sin 2\theta) - 2\theta \cos \theta - \pi \sin^2 \theta).$$

Finally, we obtain the relation

$$(A.14) \quad \psi_\xi(\xi_\infty, \theta) + \frac{2\tau}{\xi_\infty^3} \left\{ \frac{4}{\pi} \sum_{n=1}^{\infty} \lambda_n \sin \lambda_n \theta \int_0^{\pi/4} (\psi(\xi_\infty, \theta)/(\tau/\xi_\infty^2) - 1) \sin \theta d\theta \right. \\ \left. + 1 + 2 \sin 2\theta + \frac{2}{\pi} (2\theta \cos \theta - \sin 2\theta \ln(2 \sin 2\theta)) \right\} = 0,$$

which constitutes the boundary condition at ξ_∞ if $\theta = O(1)$. The corresponding relation for $\theta \ll 1$ can be easily obtained from the boundary layer solution (A.8).

Solution of the inner problem. To determine the ignition time τ_0 , it is required to find the dependence of the solution of (A.1), (A.4), $\psi(\tau)$, on the parameter τ through the solution branch $[\|\psi\|, \tau]$. Therefore we must solve the nonlinear inner problem for some values of τ . This can be accomplished by using the Newton-Kantorovich method for each fixed value of τ as follows. If $\psi^{(m)}$ is an approximation to the solution of (A.1), (A.4), the next approximation $\psi^{(m+1)} = \psi^{(m)} + \delta\psi^{(m)}$ is obtained by solving the linear problem

$$(A.15) \quad -G_\psi[\psi^{(m)}, \tau] \delta\psi^{(m)} = G[\psi^{(m)}, \tau],$$

where $G[\psi, \tau]$ is the nonlinear operator $\Delta\psi + \tau e^{\psi - (1/2)\xi^2 \sin 2\theta}$ and $G_\psi[\psi, \tau]\delta\psi$ is the linear one $\Delta\delta\psi + \tau e^{\psi - (1/2)\xi^2 \sin 2\theta} \delta\psi$. As is well known, this method converges very quickly if a good initial approximation $\psi^{(0)}$ is available; this leads to the continuation methods where we start with a known solution and then march in small steps in a continuation parameter. Although in our problem the natural marching parameter is τ , it is not the better choice because, from the typical behaviour of the reactive-diffusive systems, τ_0 is expected to be a turning point in which the Jacobian $G_\psi[\psi, \tau_0]$ becomes singular. Consequently, near τ_0 , both continuation and Newton methods fail. As is known (see, e.g., Boyd [19]), the simplest way of dealing with a turning point is to use the parameter exchange method, whose key idea is to observe that $\|\psi\|(\tau)$ is a double-valued function, but its inverse $\tau(\|\psi\|)$ is single valued. This method suggests using $\|\psi\|$ as continuation parameter instead of τ , which becomes now an unknown; i.e., the solution branch is parameterized in terms of $\|\psi\|$ instead of τ . Given a value of $\|\psi\| = \lambda$ and initial approximations $\psi^{(0)}$ and $\tau^{(0)}$, both the function ψ , such that $\|\psi\| = \lambda$, and the value of τ that satisfy (A.1), (A.4) are determined by the sequence of approximations $\psi^{(k+1)} = \psi^{(k)} + \delta\psi^{(k)}$ and $\tau^{(k+1)} = \tau^{(k)} + \delta\tau^{(k)}$ ($k = 0, 1, 2, \dots$) obtained by solving the following sequence of linear problems:

$$(A.16) \quad -G_\psi[\psi^{(k)}, \tau^{(k)}] \delta\psi^{(k)} - G_\tau[\psi^{(k)}, \tau^{(k)}] \delta\tau^{(k)} = G[\psi^{(k)}, \tau^{(k)}],$$

$$(A.17) \quad \delta\psi^{(k)}(\xi, 0) = \delta\psi_\theta^{(k)}(\xi, \pi/4) = \delta\psi_\xi^{(k)}(\xi_\infty, \theta) = 0,$$

$$(A.18) \quad \|\psi^{(k)} + \delta\psi^{(k)}\| = \lambda.$$

The continuation method begins in $\lambda \ll 1$, i.e., $\tau \ll 1$, whose corresponding solution is obtained from the linear equation $\Delta(\psi/\tau) + \exp[-\frac{1}{2}\xi^2 \sin 2\theta] = 0$.

Problem (A.16)–(A.18) is discretized using a finite volume method with a nonuniform mesh. The finest grid spacing is located around $\theta = 0$ (boundary layer) and $\xi = 0$ (where there exists a weak singularity as in the equation $\Delta\psi = -1$ [20, p. 43]). For each value of $\|\psi\|$, we solve the linear equation system for $\delta\psi$ and $\delta\tau$, obtaining, after a certain number of iterations, τ and the values of ψ at the nodes. More details about the algorithm are given in [5].

Acknowledgment. C. Vázquez-Espí thanks Professor J. M. Vega for his helpful comments.

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