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Transient Ignition of a Combustible by a Hot Body

T. Y. Xiong* and C. K. Law†
Northwestern University, Evanston, Illinois

The ignition and ignitability characteristics of a combustible mixture by a hot body of finite dimension and thereby heat capacity is studied by using matched asymptotic analysis in the limit of large activation energy, allowing for reactant consumption and the gradual cooling down of the body. It is shown that the system is governed by only a few parametric groupings whose physical significance is discussed. Furthermore, a set of universal ignitability limit curves can be identified for a given fuel-oxidizer system, allowing for generalized representation and exploration.

Nomenclature

B = frequency factor
c_p = specific heat
D = mass diffusivity
E = activation energy
ℓ = half of the slab thickness
p = pressure
Q = chemical heat release per unit mass fuel reacted
R^0 = universal gas constant
T = temperature
T_a = activation temperature (E/R^0)
W = molecular weight
$\bar{W}$ = average molecular weight
x = direction normal to the surface
Y = species mass fraction
α = thermal conductivity
λ = heat conductivity
ν = stoichiometric molar coefficient
ρ = density
σ = stoichiometric oxidizer-to-fuel mass ratio ($W_O\nu_O/W_F\nu_F$)

Subscripts

F = fuel
f = frozen state
g = gas phase
O = oxygen
s = solid phase
w = wall
0 = initial state
∞ = ambience

Introduction

THE transient ignition process of a combustible mixture by an isothermal body of constant temperature T_w has been studied[1] using matched asymptotic analysis in the realistic limit of large activation energy for the gas-phase reactions. This analysis leads to the identification of a transient Damköhler number Δ, which has an explicit linear dependence on the time t (i.e., $\Delta \sim t$), such that ignition is expected to occur when

$$\Delta = 1 \tag{1}$$

Relation (1) shows that ignition is always possible given sufficient time.

The above result is useful for highly reactive systems in which ignition occurs fairly rapidly. However, for those less reactive systems in which either the ignition source is only moderately hot and/or the reactant concentrations are low, then at least two other limitations need to be considered. The first is the relatively substantial amount of reactant consumption needed to initiate the ignition thermal runaway. The second is the gradual cooling down of the ignition source due to its finite dimension and thereby heat capacity. For these situations the criterion given by Eq. (1) becomes either inaccurate or completely inoperative in that ignition may not even occur at all.

In the present study we have removed these two limitations by first extending the transient gas-phase ignition analysis of Ref. 1 to include reactant consumption[2]; the gas-phase results are then coupled to the heat transfer process in the solid. The final result is sufficiently simple both in its parametric specification as well as numerical computation such that a reasonably general exploration of the system behavior can be conducted. In this regard we also note the worthwhile contribution of Ref. 3 in which a similar problem, with the further physical simplification that the solid temperature is spatially uniform but temporally varying, was solved completely numerically. The present study offers additional insights into the ignition behavior, the proper parametric groupings, and certain limiting conditions. A more extensive discussion on the background regarding ignition of premixtures by hot surfaces can be found in Ref. 4.

Formulation

For demonstration the infinite slab with thickness 2ℓ with the symmetry plane located at $x=0$ is chosen as the model configuration. Extension of the present analysis to the physically more relevant situation of a hot spherical particle is straightforward.

Thus, at $t=0$ the slab with initial temperature $T_0(x)$ is placed in a stagnant homogeneous combustible mixture with uniform temperature T_∞ and species mass fractions $Y_{i\infty}$. Subsequently, the mixture is heated by the slab which is cooling down simultaneously. Therefore, it is clear that the mixture may be ignited only under certain favorable situations depending on, for example, the thickness and the initial temperature of the slab, as well as the thermal and chemical properties of the mixture. We are interested in determining the ignition conditions and the associated delay period.

We first express the gas-phase temperature distribution in the reaction region next to the surface as

$$\tilde{T}_g(\tilde{x},\tilde{t}) = \tilde{T}_{gf}(\tilde{x},\tilde{t}) + \epsilon\theta(\chi;\tilde{t}) + \mathcal{O}(\epsilon^2) \tag{2}$$

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*Ph.D. Candidate, Department of Mechanical and Nuclear Engineering.

†Professor, Department of Mechanical and Nuclear Engineering; presently, Professor, Department of Mechanical Engineering, University of California, Davis, California. Associate Fellow AIAA.

where $\tilde{T} = c_p T/Q$, $\tilde{x} = x/\ell$, and $\tilde{t} = (\alpha_s/\ell^2)t$. Furthermore $T_{gf}(x,t)$ is the temperature distribution in the absence of chemical reaction, $\epsilon\theta(\chi;t)$ the corresponding temperature increase due to weak chemical reaction leading to ignition, ϵ the small expansion parameter given by $\epsilon = \tilde{T}_{wf}^2/\tilde{T}_a$, $\chi = (\tilde{T}_{wf} - \tilde{T}_\infty)\xi/\epsilon$ the stretched independent variable in the reaction region with $\chi = 0$ corresponding to the slab surface, and $\xi = \mathrm{erf}(\eta)$ with

$$\eta = \int_1^x \rho \mathrm{d}x / (2\rho_\infty^2 D_\infty t)^{1/2}$$

The ignition analysis then involves the determination of $\theta(\chi;\tilde{t})$ and the situation under which a weakly reactive state as given by Eq. (2) cannot exist.

Equation (2) also indicates that t appears only as a parameter for the function θ. Therefore, due to the large activation energy nature of the chemical reaction, the reaction is concentrated in a thin layer, next to the surface, which has the highest temperatures. Consequently, diffusion and reaction dominate in this layer, making the flow properties there locally similar in that the temporal variations are manifested parametrically instead of differentially.[1]

Following the same derivation procedure as in Ref. 1, but allowing for reactant consumption as well as varying wall temperature, it can be shown that the temperature gradient at the gas side of the slab surface is given by

$$\left(\frac{\partial \tilde{T}_g}{\partial \tilde{x}}\right)_{\pm 1} = \left(\frac{\partial \tilde{T}_{gf}}{\partial \tilde{x}}\right)_{\pm 1} + \left(\frac{2}{\pi \tilde{t}}\right)^{1/2} \left[\frac{\tilde{T}_\infty (\tilde{T}_{wf} - \tilde{T}_\infty)}{\tilde{T}_w}\right] \times \left(\frac{\alpha_s}{\alpha_\infty}\right)^{1/2} \left(\frac{\mathrm{d}\theta}{\mathrm{d}\chi}\right)_0 \tag{3}$$

where

$$\left(\frac{\mathrm{d}\theta}{\mathrm{d}\chi}\right)_0 = 1 - [1 - \Delta e^{\theta(0)}]^{1/2} \tag{4}$$

$$\begin{aligned}\Delta = {} & t\frac{\pi \epsilon B}{(\tilde{T}_{wf} - \tilde{T}_\infty)^2} \left(\frac{p\bar{W}}{R^0}\right)^{(a_\mathrm{O} + a_\mathrm{F} - 1)} \\ & \times \left(\frac{\sigma^{a_\mathrm{O}} \nu_\mathrm{F} W_\mathrm{F}}{W_\mathrm{O}{}^{a_\mathrm{O}} W_\mathrm{F}{}^{a_\mathrm{F}}}\right) T_w^{(1 + a_T - a_\mathrm{O} - a_\mathrm{F})} \\ & \times \left[\tilde{Y}_{\mathrm{O}\infty} - (\tilde{T}_{wf} - \tilde{T}_\infty)\left(\frac{\mathrm{d}\theta}{\mathrm{d}\chi}\right)_0\right]^{a_\mathrm{O}} \\ & \times \left[Y_{\mathrm{F}\infty} - (\tilde{T}_{wf} - \tilde{T}_\infty)\left(\frac{\mathrm{d}\theta}{\mathrm{d}\chi}\right)_0\right]^{a_\mathrm{F}} \exp(-\tilde{T}_a/\tilde{T}_{wf})\end{aligned} \tag{5}$$

and $\tilde{Y}_{\mathrm{O}\infty} = Y_{\mathrm{O}\infty}/\sigma$.

The above gas-phase solutions are expressed in terms of the surface temperature $\tilde{T}_w(t) = \tilde{T}_{wf}(t) + \epsilon\theta(0)$, which is to be determined from the temperature distribution within the solid, governed by

$$\frac{\partial \tilde{T}_s}{\partial \tilde{t}} = \frac{\partial^2 \tilde{T}_s}{\partial \tilde{x}^2}, \quad \tilde{T}_s(\tilde{x},0) = \tilde{T}_0(\tilde{x})$$

$$\tilde{T}_s(1,\tilde{t}) = \tilde{T}_w(\tilde{t}), \quad \frac{\partial \tilde{T}}{\partial \tilde{x}}(0,\tilde{t}) = 0 \tag{6}$$

The solution of Eq. (6) is simply

$$\tilde{T}_s(\tilde{x},\tilde{t}) = \tilde{T}_w(\tilde{t}) - 2\sum_{n=0}^{\infty} \frac{(-1)^n}{\lambda_n} e^{-\lambda_n^2 \tilde{t}} \cos\lambda_n \tilde{x} \times \left[(-1)^n \int_0^1 \tilde{T}_0'(\tilde{x}) \sin\lambda_n \tilde{x} \mathrm{d}\tilde{x} + \int_0^{\tilde{t}} e^{\lambda_n^2 \tau} \left(\frac{\mathrm{d}\tilde{T}_w}{\mathrm{d}\tau}\right) \mathrm{d}\tau\right] \tag{7}$$

where the eigenvalue $\lambda_n = (n + 1/2)\pi$.

Finally, requiring continuity of heat flux across the surface,

$$\left(\lambda_s \frac{\partial \tilde{T}_s}{\partial \tilde{x}}\right)_{\pm 1} = \left(\lambda_g \frac{\partial \tilde{T}_g}{\partial \tilde{x}}\right)_{\pm 1} \tag{8}$$

and using Eqs. (3) and (7), we obtain

$$\begin{aligned}&\sum_{n=0}^{\infty} e^{-\lambda_n^2 \tilde{t}} \left[(-1)^n \int_0^1 \tilde{T}_0'(\tilde{x}) \sin\lambda_n \tilde{x} \mathrm{d}\tilde{x} + \int_0^{\tilde{t}} e^{\lambda_n^2 \tau} \left(\frac{\mathrm{d}\tilde{T}_w}{\mathrm{d}\tau}\right) \mathrm{d}\tau\right] = -\left(\frac{\lambda_g}{\lambda_s}\right) \left(\frac{\alpha_s/\alpha_\infty}{\pi \tilde{t}/2}\right)^{1/2} \\ &\times \left(\frac{\tilde{T}_{wf} - \tilde{T}_\infty}{\tilde{T}_w}\right) \tilde{T}_\infty [1 - \Delta e^{\theta(0)}]^{1/2}\end{aligned} \tag{9}$$

In the absence of chemical reaction, Eq. (9) degenerates to

$$\sum_{n=0}^{\infty} e^{-\lambda_n^2 \tilde{t}} \left[(-1)^n \int_0^1 \tilde{T}_0'(\tilde{x}) \sin\lambda_n \tilde{x} \mathrm{d}\tilde{x} + \int_0^{\tilde{t}} e^{\lambda_n^2 \tau} \left(\frac{\mathrm{d}\tilde{T}_w}{\mathrm{d}\tau}\right) \mathrm{d}\tau\right] = -\left(\frac{\lambda_g}{\lambda_s}\right) \left(\frac{\alpha_s/\alpha_\infty}{\pi \tilde{t}/2}\right)^{1/2} \left(\frac{\tilde{T}_{wf} - \tilde{T}_\infty}{\tilde{T}_w}\right) \tilde{T}_\infty \tag{10}$$

Using Eqs. (9) and (10), $\tilde{T}_{wf}$ and $\theta(0;\tilde{t})$ can be determined. The problem is completely solved at this stage.

Much insight on the ignition behavior can be gained by simply inspecting the above relations. First, note that the right-hand side of Eq. (9) is always negative. The ignition behavior then depends on the initial temperature distribution $\tilde{T}_0(\tilde{x})$. If $\mathrm{d}\tilde{T}_0(\tilde{x})/\mathrm{d}\tilde{x} > 0$, as in the situations where the hot particle is produced through abrasion or where it is initially heated up through surface catalysis, then the first term on the left-hand side of Eq. (9) is always positive. Thus, in order for Eq. (9) to balance, we must have $\mathrm{d}\tilde{T}_w/\mathrm{d}\tilde{t} < 0$ for all $\tilde{t}$. The ignition criterion is then simply given by the vanishing of the radical term, or

$$[\Delta e^{\theta(0)}]_I = 1 \tag{11}$$

which corresponds to the S-curve ignition criterion. At the state of Eq. (11), we also have

$$\left(\frac{\partial \tilde{T}_g}{\partial \tilde{x}}\right)_{\pm 1} = \left(\frac{\partial \tilde{T}_s}{\partial \tilde{x}}\right)_{\pm 1} = 0 \tag{12}$$

which is just the adiabaticity ignition criterion of van't Hoff generalized to include heat transfer in the solid. Equation (11) also specializes to Eq. (1) for an isothermal body of constant temperature, for which $\theta(0) = 0$, as it should be.

On the other hand, if $\mathrm{d}\tilde{T}_0(\tilde{x})/\mathrm{d}\tilde{x} < 0$, as in the situation where a molten particle is cooling down, the first term of Eq. (9) is always negative. Then at the S-curve ignition state we must have $\mathrm{d}\tilde{T}_w/\mathrm{d}\tilde{t} > 0$. However, since $\mathrm{d}\tilde{T}_w(0)/\mathrm{d}\tilde{t} < 0$ initially, a state satisfying

$$\left(\frac{\mathrm{d}\tilde{T}_w}{\mathrm{d}\tilde{t}}\right) = 0 \tag{13}$$

is attained before the state of Eq. (11). Physically, at the state of Eq. (13) there is sufficient chemical heat release and accumulation that the slab now starts gaining energy from the gas. Therefore, in terms of reaction being self-sustaining, Eq. (13) is an earlier indication of the attainment of ignition than Eq. (11).

In the special case of an initially uniform slab temperature, it can be easily shown that Eqs. (11-13) are equivalent to each other. Furthermore, the slab temperature also becomes uniform at ignition, that is,

$$\tilde{T}_s(\tilde{x},\tilde{t}_I) = \tilde{T}_w(\tilde{t}_I) \tag{14}$$

Results

$\tilde{T}_w(\tilde{t})$ may be presented as functions of the five system parameters, namely, $\tilde{T}_a$, $\tilde{T}_0$, $\tilde{T}_\infty$,

$$A = \left\{ \frac{(\lambda c_p \rho)_g}{(\lambda c_p \rho)_s} \right\}^{1/2}$$

and

$$Da = \frac{B\ell^2}{\alpha_s \tilde{T}_a}\left(\frac{p\bar{W}}{R^0}\right)^{(a_O + a_F - 1)} \times \left(\frac{Q}{c_{pg}}\right)^{(1 + a_T - a_O - a_F)} \tilde{Y}_{O\infty}{}^{a_O}\, \tilde{Y}_{F\infty}{}^{a_F} \left(\frac{\sigma^{a_O}\nu_F W_F}{W_O{}^{a_O} W_F{}^{a_F}}\right) \times \exp\left(-\frac{\tilde{T}_a}{\tilde{T}_0}\right)$$

For simplicity only the case of an initially isothermal slab will be studied. Equation (9) can now be expressed as

$$\sum_{n=0}^{\infty} \int_0^{\tilde{t}} e^{-(n+1/2)^2\pi^2(\tilde{t}-\tau)} \left(\frac{d\tilde{T}_w}{d\tau}\right) d\tau = -A\left(\frac{2}{\pi \tilde{t}}\right)^{1/2} \frac{\tilde{T}_\infty(\tilde{T}_{wf} - \tilde{T}_\infty)}{\tilde{T}_w}[1 - \Delta e^{\theta(0)}]^{1/2} \tag{15}$$

where

$$\Delta e^{\theta(0)} = \Delta \exp\left[\frac{\tilde{T}_a}{\tilde{T}_{wf}}\left(\frac{\tilde{T}_w}{\tilde{T}_{wf}} - 1\right)\right] \tag{16}$$

The parameters A and Da have the following physical meaning. First, A is the thermal responsivity of the system, representing the relative magnitudes of the thermal properties of the mixture and the hot body. As $A \to 0$, the body temperature tends to remain both uniform, because of its high thermal conductivity, and constant, because of its high thermal capacity. Consequently, the body behaves as a constant ignition source, which is the case treated in Ref. 1. However, with increasing A, the body temperature is more susceptible to change, the ignition process becomes more transient, and the ignition delay is longer as the body gradually cools down. Allowance for reactant consumption of course causes further delay in the onset of ignition.

The parameter Da is a Damköhler number representing the ratio of the characteristic diffusion time (ℓ^2/α_g) to the characteristic reaction time. Hence the system would be more ignitable with increasing Da.

The final point to note is that the effect of geometry of the body, which was shown to be only of secondary importance for the isothermal body,[1] asserts a stronger influence in the present situation because it affects the rate with which the body loses heat to the ambience and consequently the values of T_{wf}.

Results were obtained for representative values of hydrocarbon/air reactions. Figure 1 shows profiles of the slab temperature with and without chemical reaction in the gas phase. As anticipated, the presence of chemical reaction slows down the decrease in the slab temperature. At ignition the slab temperature becomes uniform.

Figure 2 shows the sensitivity of the ignition factor $\Delta e^{\theta(0)}$ to variations in the initial slab temperature $\tilde{T}_0$, where $C = Da/\exp(-\tilde{T}_a/\tilde{T}_0)$. It is seen that small changes in $\tilde{T}_0$ not

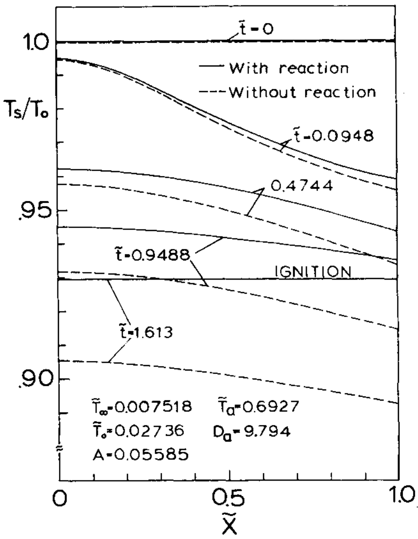

Fig. 1 Development of the temperature profiles within the slab with and without gas-phase reaction.

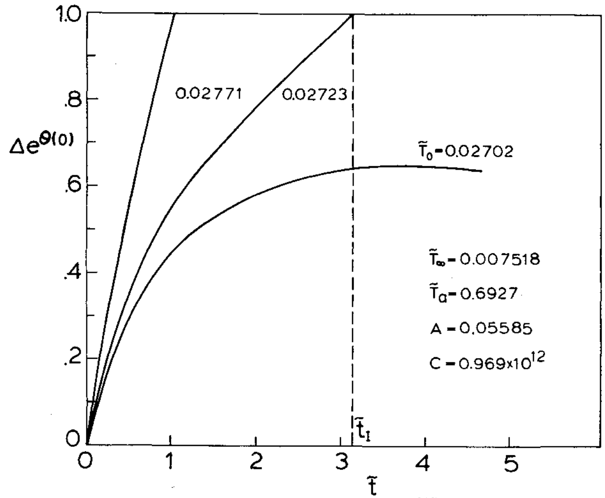

Fig. 2 Development of the ignition factor $\Delta e^{\theta(0)}$ to demonstrate the ignitable and nonignitable situations.

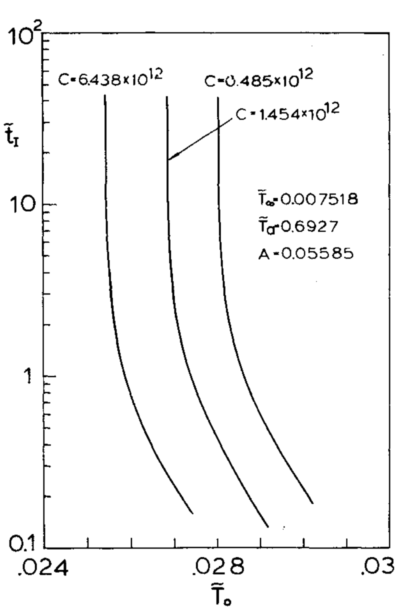

Fig. 3 Typical ignition delay plots to demonstrate the existence of absolute ignition limits.

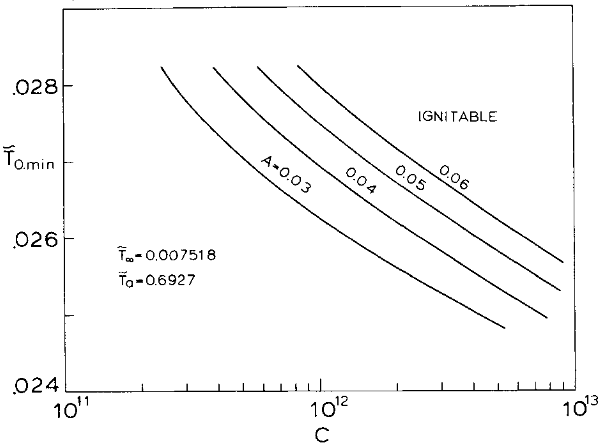

Fig. 4 General ignitability curves for the given set of kinetic parameters.

only can delay the onset of ignition significantly, but it can also render the system to be unignitable.

Figure 3 illustrates the dependence of the ignition delay on $\tilde{T}_0$. It is clear that for given A and C there exists a minimum $\tilde{T}_0$, $\tilde{T}_{0,\min}$, below which ignition is not possible. Figure 4 then plots $\tilde{T}_{0,\min}$ as functions of A and C. Thus states above the curves are ignitable while those below them not ignitable. Figure 4 can be considered to be a general ignitability plot for specified fuel and oxidizer, and thereby the related kinetic constants.

Conclusions

In the present study the ignition and ignitability characteristics of a combustible mixture by a hot slab which is cooling down during the ignition delay because of its finite heat capacity have been identified. Different ignition responses and criteria exist for the slab whose surface temperature is initially hotter or colder than that of the interior. A set of general ignitability limit curves can also be generated for a fuel-oxidizer system.

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