On the calculation of the minimum ignition energy

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1. Introduction

The success of the initiation of a deflagration by an external energy source depends on the competition of heat conduction and radical diffusion with chemical heat release. As an order-of-magnitude criterion, one may state that the minimum ignition energy

$$E_m \sim \rho_o c_{p_o} T_o \delta_l^3 \quad (1)$$

is associated with conditions such that the heat release increases the temperature by a factor of order unity in a hot pocket of size comparable to the laminar flame thickness $\delta_l \sim \alpha_o/v_l$. Here, T_o , ρ_o , c_{p_o} , and α_o are the initial values of the temperature, T , density, ρ , specific heat at constant pressure, c_p , and thermal diffusivity for the gas mixture, and v_l is the corresponding laminar-flame propagation velocity. It should be noted that, although the criterion given in Eq. (1) is valid under most conditions, departures are sometimes observed [1,2].

For symmetric sources, the accurate computation of E_m involves the integration of transient-one-dimensional conservation equations with detailed chemistry and transport phenomena. For given mixture conditions, the resulting E_m depends on the characteristics of the energy source, decreasing for decreasing values of the size r_d of the region where heat is deposited [3,4], so that the most effective sources are concentrated sources with $r_d \ll \delta_l$.

The other fundamental parameter that defines the external energy source is the duration of the deposition period, t_d . When t_d is of the order of the chemical

time $t_l = \alpha_o/v_l^2$, defined as the time characteristic of conductive heat propagation across the flame, both heat conduction and chemical reaction are seen to occur simultaneously during the deposition period. The associated thermal expansion induces outward velocities of order v_l , with a characteristic Reynolds number of order unity, which are much smaller than the velocity of sound of the reference state $a_o \sim 10^3 v_l$. As a result, the pressure variations from its ambient value are negligibly small, giving a near-isobaric flow that has been analyzed in [5] for the nonreacting case. As seen in Fig. 1, under these near-isobaric conditions the value of E_m corresponding to a concentrated energy source decreases for decreasing values of t_d .

The result is modified for t_d of the order of the acoustic time scale for propagation of pressure disturbances across the hot pocket $t_a = \delta_l/a_o \ll t_l$, when the flow during the deposition period is characterized by relative pressure differences of order unity and by the appearance of a shock wave that heats up the mixture as it propagates outward [6], distributing in an extended far-field region a significant fraction of the energy deposited, which becomes larger as the shock becomes stronger for smaller values of t_d/t_a . Since the associated temperature increment in this far-field region is relatively small, the contribution of this fraction of energy to the ignition process is only marginal. As a result, the value of E_m increases for decreasing values of t_d/t_a , toward the limiting value corresponding to instantaneous heat release ($t_d \ll t_a$).

The considerations given above indicate that the smallest value of E_m is achieved by concentrated sources of deposition size $r_d \ll \delta_l$ and with a deposition time in the intermediate range $t_a \ll t_d \ll t_l$. Two distinct periods can be identified in the resulting near-isobaric flow evolution: a deposition period for times of the order of t_d , in which the effect of the chemical heat release on the temperature is negligible, and the subsequent ignition period

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Fig. 1. The variation of the minimum ignition energy with the deposition time t_d for a stoichiometric hydrogen–air mixture at atmospheric pressure and $T_0 = 300$ K as obtained by integration of the near-isobaric conservation equations for a line source (upper plot) and a point source (lower plot) of constant heating rate; the dashed lines indicate the value of E_m corresponding to a source with $t_a \ll t_d \ll t_1$, determined with use made of Eq. (10) to evaluate the initial temperature profile. The insets show the self-similar profiles $G(r/r_h)$ corresponding to $\sigma = 0.7$.

for times of order t_1 , which proceeds with no external heating. Consideration is given below to the solution emerging for times in the intermediate period $t_1 \gg t \gg t_d$, when the temperature exhibits a self-similar distribution that scales with the amount of energy deposited but it is otherwise independent of other energy source characteristics such as deposition size, deposition time, and heating-rate variation. This self-similar profile enters as initial conditions for the temperature when integrating the energy conservation equation during the ignition period, thereby providing a simple calculation procedure for the minimum ignition energy that circumvents numerical stiffness. To obtain the solution, we start by formulating in the following section the problem corresponding to flame initiation by a concen-

trated external energy source in the distinguished limit $t_d \sim t_1$.

2. Near-isobaric deflagration initiation by symmetric energy sources

In the limit $t_d \sim t_1$, the relative pressure variations that appear are negligibly small, of order $(v_1/a_0)^2$. When these are neglected in the equation of state the momentum balance equation becomes secondary for the computation of the resulting initiation events, which requires integration of the well-known one-dimensional transient continuity, energy, and species conservation equations. The initial conditions for the problem can be written as

$$t = 0: \quad \rho = \rho_0, \quad T = T_0, \quad Y_i = Y_{i0} \quad (2)$$

while the boundary conditions for $t > 0$ are

$$r = 0: \quad u = 0, \quad 2^j \pi r^j k \frac{\partial T}{\partial r} = -\frac{E_j}{t_d} q(t), \quad \frac{\partial Y_i}{\partial r} = 0 \quad (3)$$

and

$$r = \infty: \quad T = T_0, \quad Y_i = Y_{i0}, \quad (4)$$

where u , Y_i , r , and t represent, respectively, the velocity, mass fraction of species i , radial coordinate, and time. The index j is used to denote the point source ($j = 2$) and the line source ($j = 1$). Correspondingly, the energy of the point source E_2 and the energy per unit length of the line source E_1 are used to define a dimensionless heating rate of order unity $q = q'/(E_j/t_d)$, which must satisfy $\int_0^{t_d} q dt = t_d$ and vanishes for $t \geq t_d$. This definition yields, for instance, $q = 1$ for the source of constant rate used in the integrations reported below.

To determine E_m for a given value of t_d one needs to integrate the problem stated above for increasing values of E_j , until a deflagration successfully develops. Results of the integrations for a stoichiometric hydrogen–air mixture at atmospheric pressure and $T_0 = 300$ K are given in Fig. 1. The so-called San-Diego mechanism was used for the detailed chemistry description [7], while $c_p = \sum_{i=1}^N c_{pi} Y_i$ was computed with use made of the NASA polynomial fits for $c_{pi}(T)$, and the approximate law $(k/k_0) = (c_p/c_{p0})(T/T_0)^\sigma$ with $\sigma = 0.7$ was employed to compute the changes in thermal conductivity k from its initial value k_0 , a widely used approximation that gives accurate results for flame calculations [8]. As can be seen in the figure, the value of E_m decreases as t_d/t_1 decreases, confirming that the minimum ignition energy is achieved for deposition times in the

range $t_a \ll t_d \ll t_l$. The computation of ignition for such short deposition times is complicated by the appearance of large temperature gradients in the hot kernel during the deposition period. To circumvent these difficulties, we address below the solution for $t \ll t_l$, providing as a key result the self-similar temperature distribution that appears for $t_d \ll t \ll t_l$.

3. Heat deposition for $t_a \ll t_d \ll t_l$

In the analysis of the deposition period for $t_d \ll t_l$, one can neglect the chemical heat release, which would give a negligible contribution to the energy balance, along with changes in molecular weight for the hot gas mixture, a simplification that applies in combustion of fuel-air mixtures, reducing the ideal gas law to $\rho T = \rho_o T_o$. Furthermore, the specific heat within the hot kernel reaches at high temperature a constant value c_{ph} , which can be used when writing the energy equation in the conservative form

$$\frac{\partial}{\partial t}(\rho c_{ph} T) + \frac{1}{r^j} \frac{\partial}{\partial r} \left[r^j \left(\rho u c_{ph} T - k \frac{\partial T}{\partial r} \right) \right] = 0, \quad (5)$$

where viscous dissipation and conductive heat transport by diffusion have been discarded. Since $\rho T = \rho_o T_o$, a first integral of Eq. (5) with use made of Eq. (3) provides

$$2^j \pi r^j \left(\rho_o c_{ph} T_o u - k \frac{\partial T}{\partial r} \right) = \frac{E_j}{t_d} q(t), \quad (6)$$

which can be substituted into the continuity equation to finally yield

$$\frac{\partial}{\partial t} \left(\frac{2^j \pi \rho_o c_{ph} T_o}{T} \right) + \frac{1}{r^j} \frac{\partial}{\partial r} \left[\frac{1}{T} \left(2^j \pi r^j k \frac{\partial T}{\partial r} + \frac{E_j}{t_d} q \right) \right] = 0. \quad (7)$$

The temperature during the deposition period is determined by integrating the above equation with the initial and boundary conditions given in Eqs. (2)–(4). For the following development it is useful to write the first quadrature

$$\int_0^\infty 2^j \pi \rho c_{ph} (T - T_o) r^j dr = E_j \frac{\int_0^t q dt}{t_d}, \quad (8)$$

which indicates that the energy deposited up to time t , $E_j \int_0^t q dt / t_d$, appears in the hot pocket as an enthalpy increment.

As seen in [5], in the limit $t_d \ll t_l$ the thermal wave determined by integration of Eq. (7) becomes a front solution in which the hot core surrounding the source, which is nearly empty, remains distinct from the outer

cold gas, at temperature $T = T_o$. The location of the contact surface, r_h , that separates the hot core from the outer cold gas is determined by the equation $[2^j \pi / (j+1)] \rho_o c_{ph} T_o r_h^{j+1} = E_j (\int_0^t q dt / t_d)$, as follows from Eq. (8) by introducing $T/T_o \gg 1$ for $r < r_h$ and $T = T_o$ for $r > r_h$. Thus the hot core grows as dictated by the heating rate until the external heating ends at $t = t_d$, and the separating contact surface remains stagnant for $t > t_d$, with a final radius given by

$$E_j = \frac{2^j \pi}{j+1} \rho_o c_{ph} T_o r_h^{j+1}. \quad (9)$$

The temperature within the hot core continuously decreases for $t > t_d$, reaching rapidly the self-similar form [6]

$$\frac{T - T_o}{T_o} = \left(\frac{r_h^2 / \alpha_o}{t} \right)^{1/(\sigma+1)} G \left(\frac{r}{r_h} \right), \quad (10)$$

whose time dependence can be anticipated from a simple order-of-magnitude balance in the governing equation (7). The function G is determined by integrating $1/(\sigma+1) + G(\eta^j G^{\sigma-1} G_\eta)_\eta / \eta = 0$ with boundary conditions $G_\eta(0) = G(1) = 0$, where the subscript η denotes differentiation with respect to the variable $\eta = r/r_h$ [6]. In deriving the above equation from Eq. (7), the thermal conductivity has been written in the constant-specific-heat approximation $k/k_o = (c_{ph}/c_{po})(T/T_o)^\sigma$. The profiles $G(r/r_h)$ corresponding to $\sigma = 0.7$ for $j = (1, 2)$, to be used in connection with Eq. (10), are shown as insets in Fig. 1.

4. The simplified calculation procedure

Use of Eq. (10) evaluated at $t_i \ll r_h^2 / \alpha_o$ as initial condition for the temperature and density $\rho/\rho_o = (T/T_o)^{-1}$ in integrating the continuity and energy equations removes the necessity to consider the deposition period. Correspondingly, the boundary condition for the temperature at the source is replaced in the integration by the symmetry condition $\partial T / \partial r = 0$. Although significant dissociation occurs during the deposition period, these composition changes need not be considered due to the relatively small energy involved, so that one may assume that the initial composition is given by $Y_i = Y_{io}$ at $t = t_i$. With this simplified initial condition, dissociation is seen to occur in the hot pocket immediately after the numerical integration is started, so that the composition adjusts rapidly to that present at the end of the deposition period.

The proposed set of initial and boundary conditions circumvents the numerical difficulties associated with the limit of concentrated energy sources in

the regime $t_d \ll t_l$. To determine the minimum ignition energy, successive integrations with increasing values of r_h must be considered, until critical conditions for deflagration initiation are reached. For instance, for the stoichiometric hydrogen–air mixture considered in Fig. 1, the critical r_h for ignition is $r_h = 0.71 \times 10^{-4}$ m for $j = 1$ and $r_h = 1.48 \times 10^{-4}$ m for $j = 2$. Once the critical value of r_h is determined, use of Eq. (9) provides the minimum ignition energy for a given fuel–air mixture. The result depends on the value of the specific heat at high temperature c_{ph} used in the computation, although the resulting E_m is not critically dependent on this choice provided a sufficiently large temperature is selected for evaluating c_{ph} . For the values computed here, which are represented by dashed lines in Fig. 1, the specific heat was evaluated at $T = 5000$ K, a selection that yields $E_m = 0.00931$ J/m for $j = 1$ and $E_m = 6.03 \times 10^{-6}$ J for $j = 2$.

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