AN ANALYSIS OF LEWIS NUMBER AND FLOW EFFECTS ON THE IGNITION OF PREMIXED GASES

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We have analysed numerically the ignition of a combustible gas to which heat is added over a specified period at a spherical boundary of small diameter. We solve conservation equations for reactant and sensible enthalpy and allow the gas to undergo a one step chemical reaction. The numerical technique involves a finite difference scheme with an adaptive grid. We find that, until the flame has grown beyond a critical radius, it relies upon the heat source to prevent its extinction. A minimum energy is required for successful ignition. This minimum increases as the Lewis number of the mixture increases. The minimum ignition energy also increases if the flame front is stretched. This behaviour is in very close agreement with experimental observations of the spark ignition of turbulent mixtures.

1. Introduction

To explain their observations of spark ignition Lewis and von Elbe made intuitive arguments in terms of “excess enthalpy” and “flame stretch”. Though their description provides useful scales for the minimum ignition energy and predicts its relationship with pressure and burning velocity, it does not completely define the process. To gain further insight several numerical studies have been made of ignition initiated by small, hot pockets of gas. Generally, this work has involved complex chemical kinetic schemes. Dixon-Lewis and Shepherd examined the ignition of hydrogen-air mixtures by spherical and cylindrical hot spots. They investigated the effect of pocket size and radical addition on minimum ignition energy. Overley, Overholser and Reddien studied the influence on minimum ignition energy of hot pocket size and shape; they looked at spherical and spheroidal pockets. Kailasanath, Oran and Boris included the effect of adding heat to the hot pocket over some prescribed period rather than instantaneously.

The present authors studied the ignition of a gas with a Lewis number of one, which could undergo a one step chemical reaction. We compared the effects of adding heat at a planar boundary and at cylindrical and spherical boundaries of very small diameter. Only the spherical geometry provided results which were similar to experimental observations of spark ignition: there was a minimum radius below which deceleration and extinction of a spherical flame could occur, a minimum energy for ignition, an optimum source duration and a sensitivity to imposed strain fields. The importance of spherical geometry was illuminated by the asymptotic analysis of Deshaies and Joulin. Their work reveals a minimum radius for the unsupported propagation of a spherical flame. Kailasanath and Oran and Sloane included detailed chemical kinetic schemes in their numerical studies of the ignition of hydrogen-oxygen-nitrogen mixtures and methane-oxygen-argon mixtures, but still found that flame curvature had a major influence on their results. Kailasanath and Oran observed large flame decelerations and a tendency to extinction in the spherical system, while Sloane found that spherical geometry was essential for his calculated minimum ignition energies to show the correct dependence on equivalence ratio.

In view of the importance of geometrical and physical factors it is worthwhile to investigate the effect of variation of the parameters in a model involving only a one step chemical reaction. This is the purpose of the present paper. In particular we investigate two areas: the role of an effective Lewis number in controlling the dependence of ignition energy on equivalence ratio and the possibility of modelling the influence of turbulent motion on spark ignition in terms of flame stretch.
2. The Conservation Equations and the Method of Solution

We wish to analyse the initiation of a spherical flame in a premixed gas by a small, spherical source of heat. We consider a one step reaction controlled by the concentration of one limiting reactant. The conservation equations for the mass fraction of this reactant and sensible enthalpy are:

\[
\frac{\partial \tilde{Y}}{\partial \tau} + \rho \frac{\partial \tilde{Y}}{\partial x} = \frac{1}{\hat{\rho} L C_p \tilde{x}^2} \frac{\partial}{\partial \tilde{x}} \left( \tilde{k} \frac{\partial \tilde{Y}}{\partial \tilde{x}} \right) - \frac{W}{\hat{\rho}} \tag{1}
\]

and

\[
\frac{\partial \tilde{T}}{\partial \tau} + \rho \frac{\partial \tilde{T}}{\partial x} = \frac{1}{\hat{\rho} C_p \tilde{x}^2} \frac{\partial}{\partial \tilde{x}} \left( \tilde{k} \frac{\partial \tilde{T}}{\partial \tilde{x}} \right) + \frac{QW}{\hat{\rho} C_p} \tag{2}
\]

where

\[W = \hat{\rho} B \tilde{Y} \exp \left( -\frac{E}{RT} \right) \tag{3}\]

A nomenclature is provided later. The continuity equation is:

\[
\frac{\partial \tilde{\rho}}{\partial \tau} + \rho \frac{\partial \tilde{\rho}}{\partial x} + \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \tilde{\rho} \frac{\partial \tilde{\rho}}{\partial x} \right) = 0 \tag{4}
\]

The heat addition takes place at a spherical surface with its centre at \( x = 0 \). The term \( \epsilon \) in Eq. (4) corresponds to flows in directions normal to the radial one. It leads to a velocity gradient in the radial direction of \( \epsilon/3 \) for the constant density case and a flow generated flame stretch of the same value. Such a straining flow field could be generated by a distribution of sinks on an axis of the sphere. Though such a flow field would be difficult to produce practically, it allows us to investigate the influence of flow generated flame stretch in a one dimensional problem. We shall assume \( \tilde{k}^{-1} \propto \tilde{x} \propto \tilde{T} \). Equations (1) to (4) may be non-dimensionalised by substituting:

\[
\begin{align*}
T &= \tilde{T}/\tilde{T}^*, T_o &= \tilde{T}_o/\tilde{T}^*, Y &= \tilde{Y}/\tilde{Y}_o, \\
\delta &= \tilde{\delta}/\tilde{u}_l C_p, \tau &= x/\tilde{\delta}, \epsilon &= \tilde{\epsilon}/\tilde{u}_l, R &= \tilde{T}^* - T_o,
\end{align*}
\]

where \( \tilde{u}_l \) is the adiabatic burning velocity, \( \delta \) is the adiabatic flame thickness and the tilde indicates a dimensional variable, the subscript zero indicates unburnt gas conditions, and the superscript asterisk indicates conditions in the burnt gas behind a planar, adiabatic, laminar flame. The non-dimensional conservation equations are:

\[
\begin{align*}
\frac{\partial \tilde{Y}}{\partial \tau} - \tilde{\epsilon} \frac{\partial \tilde{Y}}{\partial \psi} &= \frac{1}{L} \frac{\partial}{\partial \psi} \left( \tilde{r} \frac{\partial \tilde{Y}}{\partial \psi} \right) \\
- \beta^2 \tilde{M} \tilde{Y} \exp \beta \left( 1 - \frac{1}{T} \right) \tag{5}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial \tilde{T}}{\partial \tau} - \tilde{\epsilon} \frac{\partial \tilde{T}}{\partial \psi} &= \frac{\partial}{\partial \psi} \left( \tilde{r} \frac{\partial \tilde{T}}{\partial \psi} \right) \\
+ \frac{R\beta^2 \tilde{M}} \tilde{Y} \exp \beta \left( 1 - \frac{1}{T} \right) \tag{6}
\end{align*}
\]

We have eliminated the continuity equation by introducing the mass weighted coordinate, \( \psi \), such that:

\[
\frac{\partial \tilde{\rho}}{\partial \tau} = \tilde{r} \frac{\partial \tilde{T}}{\partial \psi} = \tilde{r} \frac{T}{T} \tag{7}
\]

The boundary conditions for the equations are set by the heat addition at the spherical surface and far field conditions. The heat addition is at a surface defined by \( \psi = a \). A small value, \( a = 0.05 \), was chosen so that the heat addition reasonably models a point source. Thus, we have:

\[
\begin{align*}
\frac{\partial \tilde{T}}{\partial \psi} &= \left( \frac{T}{T} \right)^{4/3} H(t) \text{ at } \psi = a \\
T &= T_o, \ Y = 1 \text{ at large } \psi \tag{8}
\end{align*}
\]

The term \( (T/T)^{4/3} \) is added so that a constant value of \( H \) corresponds to a constant rate of heat addition. \( H(t) \) was given the form shown in Fig. 1. The initial conditions are:

\[
T = T_o, \ Y = 1 \text{ for all } \psi \tag{9}
\]

It is straightforward to show that the total energy added is:

\[
E = 4\pi \left(3a\right)^{4/3} \int_0^\infty H(t) \ dt \tag{10}
\]

We note that the dimensional energy is:

\[
\tilde{E} = \tilde{\rho}_o C_p \delta^3 \tilde{T}^* E \tag{11}
\]
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The governing Eqs. (5), (6), (7), are discretised in space using an adaptive mesh and corresponding finite-difference approximations, to give a system of ordinary differential equations in time for $T$ and $Y$ (of order $2N$, where $N$ is the number of space points). Within certain limits the non-uniform space mesh is generated by the co-ordinate transformation:

$$X(\psi, \tau) = \frac{\int_{\psi_{i}}^{\psi} J(\psi, \tau) d\psi}{\int_{\psi_{N}}^{\psi} J(\psi, \tau) d\psi},$$  \hspace{1cm} (12)

where $J(\psi, \tau)$, the monitor function, is some measure of space derivatives of $T$ and $Y$. For a given uniform $X$ mesh $X_i = (i - 1) \Delta X, i = 1, \ldots, N$ with $(N - 1) \Delta X = 1$, constant for all time, the above transformation adapts the spacing of the corresponding $\psi_i$ points in proportion to the gradients of $T$ and $Y$. For the present problem the monitor function we use is:

$$J(\psi, \tau) = \left| \frac{\partial Y}{\partial \psi} \right| + \left| \frac{\partial T}{\partial \psi} \right|$$  \hspace{1cm} (13)

The mesh allows accuracy and fine resolution of the flame to be combined with computational efficiency. The limits on the mesh spacing are provided by user chosen criteria on maximum and minimum mesh sizes $\Delta \psi_i$. The finite-difference discretisations, space remeshing and time integration are performed automatically by the SPRINT package (Software for PRoblems IN Time) developed jointly by Leeds University and Thornton.\textsuperscript{[10]}

The calculations have been performed over a range of values of Lewis number, $L$, activation energy, $\beta$, and initial temperature, $T_i$. The initial temperature and flame temperature are easily calculated to give $T_e$. However, a wide range of values of activation energy are quoted in the literature. Lavoie\textsuperscript{[11]} gave activation energy as a function of equivalence ratio for propane-air mixtures. Though it is often assumed that activation energy is independent of concentration, his results show a strong peak at an equivalence ratio of one. The activation energy falls off faster than adiabatic flame temperature as the mixture is weakened or richened. In view of the numerous uncertainties it seems appropriate to use a constant value of non-dimensional activation energy, $\beta$, in the present work: we have performed our calculations for $\beta = 8$ and $\beta = 10$. Our results later will show that, though $\beta$ is important, it is a much less significant parameter than the Lewis number. For extremely rich and extremely weak mixtures the Lewis number should be based on the diffusivity of the deficient component. However, we require some intermediate value for other mixtures. We obtained an effective Lewis number by means of the formula derived by Joulin and Mitani\textsuperscript{[12]} in their study of the instability of two reactant flames. Their formula is:

$$L = L_2 - G (L_1 - L_2)$$  \hspace{1cm} (14)

where $L_2$ and $L_1$ are the Lewis numbers of the deficient and abundant reactants. $G$ is a function of the equivalence ratio and the orders of the reaction which we have assumed to be one with respect to both reactants. The expression is valid for $L_1$ and $L_2$ near unity. $M$, the eigenvalue of the adiabatic flame problem, is well approximated by\textsuperscript{[15]}

$$M = \frac{1}{2L} + \frac{(0.656 + L)/\beta}{G L}$$

In our previous work we found that for Lewis number, $L$, equal to unity the minimum ignition energy showed little sensitivity to the duration, $t_3$, of the heat source for $t_3$ less than one. For the present calculations we set $t_3 = 1$ except for those at large Lewis number where large energies were required and we found much longer source durations were acceptable.

### 3. Results

As indicated by Kapila\textsuperscript{[14]} and discussed in our previous paper the commencement of the heat source is followed by heating, induction, local explosion and propagation stages. Ignition failure can occur as a result of flame extinction early in the propagation stage as the flame front moves away from the source. Sets of temperature distributions illustrating a successful ignition and an extinction are shown in Figs. 2 and 3 respectively. Some position diagrams
for flames initiated in different mixtures by different heat sources are shown in Fig. 4. We have defined flame position as the point where the steepest tangent to the concentration profile that may be drawn within the flame front cuts the $Y = 0$ axis. Initially the flame propagates quickly, at a speed close to the normal burning velocity, while it is driven by the heat source. After cessation of the source the flame speed is much reduced. For each mixture there is a critical radius which the flame must reach, aided by the heat source, before it may continue unsupported. This behaviour is in qualitative agreement with the experimental observations of flame growth by Lintin and Wooding, de Soete and Akindele, Bradley, Mak and McMahon. The minimum energy for ignition increases with the critical radius.

We have investigated the influence of the parameters $T_o$, $\beta$ and $L$ on the minimum ignition energy. Figure 5 shows the dependence on $T_o$: as we might expect, the minimum ignition energy decreases as the initial temperature is brought closer to the flame temperature.
The influence is quite strong: in dimensional terms a 10°C rise in ambient temperature reduces the minimum energy for ignition by about ten per cent. Figure 6 is of greater interest: it shows how minimum ignition energy increases monotonically with Lewis number. The Lewis number is large when the mixture is very deficient in a heavy, slowly diffusing gas: it will be small when the mixture is very deficient in a light, rapidly diffusing gas. There is a transition region between the two extremes, which, for typical alkanes, occupies most of the flammable range. Thus, we should expect the equivalence ratio at which methane-air mixtures are most easily ignited to be the lowest of all the alkanes. Propane-air mixtures will have the next lowest equivalence ratio; the equivalence ratios of lowest spark ignition energy will become richer as the molecular weight of the fuel increases. This is exactly as found in experiments.1

It can be seen from Fig. 6 that the effect of increasing activation energy is to increase slightly the sensitivity of minimum ignition energy to Lewis number. This arises from the imbalance between chemical and sensible enthalpy fluxes that can occur in flames of non-unity Lewis number.18 When Lewis number is greater than one the imbalance leads to a reduction in the flame temperature compared with the unity Lewis number case. Increasing the activation energy increases the sensitivity of the flame to these temperature changes.

We have used Eq. (11) in conjunction with the data such as that listed in Table 1 to calculate dimensional minimum ignition energies for methane-air and propane-air mixtures over a range of equivalence ratios. The results are shown in Fig. 7. Although the minimum ignition energies for the most ignitable mixtures are a factor of 5 smaller than the values measured in spark ignition experiments, the curves are qualitatively correct. The difference is not unreasonable considering that our model is a spherical one taking no account of the real shape of the spark source or heat losses to the electrodes. Moreover, quite large variations may arise from small errors in the flame thickness, δ.

Finally, we have explored the influence of the strain rate term, ε, in Eqs. (5) and (6). As shown in Fig. 8 the addition of this term increases the minimum ignition energy particularly of mixtures with large Lewis numbers. This can be explained in terms of the known sensitivity of flames, especially large Lewis number flames, to strain fields. It seems likely that this sensitivity to strain rate reflects the relationship between the minimum energy for spark ignition and the root mean square, turbulent strain rate found by Tromans and O'Connor19 in their experiments on the spark ignition of turbulent mixtures. To investigate this we have replotted our theoretical curves in Fig. 9 together with the results of Tromans and O'Connor and some taken from Ballal and Lefebvre.20 All the experimental results are for cases where the smallest eddies of the turbulent motion are larger than or approximately equal to the laminar flame thickness.

The independent variable used in Fig. 9 is the rate of flame stretch, that is the increase of area of material surface in the flame front. This equals ε/3 in the numerical analysis and approximates one half of the root mean square turbulent strain rate in the experiments. The minimum ignition energy was normalised on the value at zero stretch rate. The agreement is remarkably good.

4. Discussion

Our model is restricted to one step chemistry; the combustible mixture is described only by its Lewis number, activation energy and, via the non-dimensionalization, its burning velocity and flame thickness. Omission of complex chemistry in combination with advanced numerical techniques has allowed us to perform over 300 simulations economically on a readily available computer, an IBM 4341. It has emphasised the physical aspects of the problem. Perhaps the best justification is found in the results; at least qualitative agreement with experiments is achieved without parameter fitting. The implication is that minimum spark ignition energy is mainly controlled by physical mechanisms such as flame curvature and stretch. These processes influence flame propagation through balances and gradients in the
TABLE I

Typical data used to generate Figure 7

<table>
<thead>
<tr>
<th>Mixture</th>
<th>Temperature ratio, ( T^*/T_0 )</th>
<th>Lewis number, ( L )</th>
<th>Flame thickness, ( \delta \times 10^6 ) m</th>
<th>Calculated non-dimensional minimum ignition energy, ( E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane-air</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.8</td>
<td>6.70</td>
<td>0.967</td>
<td>103</td>
<td>45.5</td>
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<td>0.9</td>
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<td>0.977</td>
<td>78</td>
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<td>63.0</td>
</tr>
<tr>
<td>1.1</td>
<td>7.42</td>
<td>1.00</td>
<td>53</td>
<td>65.1</td>
</tr>
<tr>
<td>Propane-air</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.9</td>
<td>7.31</td>
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<td>59</td>
<td>492</td>
</tr>
<tr>
<td>1.0</td>
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<td>54</td>
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</tr>
<tr>
<td>1.28</td>
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<td>1.04</td>
<td>59</td>
<td>77.5</td>
</tr>
<tr>
<td>1.40</td>
<td>6.88</td>
<td>1.00</td>
<td>69</td>
<td>56.1</td>
</tr>
</tbody>
</table>

Fig. 7. Calculated minimum ignition energies for methane-air and propane-air mixtures.

convection-diffusion zone of the flame front;\(^{18}\) they couple with the chemistry in a gross and indirect way. Lewis number will remain crucial and our present theory will be applicable so long as the sheet-like flame structure and reaction-diffusion zone are maintained.

The practical limits and possibilities of our theory remain to be tested by comparison of our predictions of ignition energy with experimental results over a range of combustible mixtures and conditions. A most exciting future application of the analysis is to the flame development period following ignition, which is vital to the performance of gasoline engines.

5. Conclusions

(i) Our numerical calculations predict the spherical flame growth and extinction that may follow heat addition to a gas.

(ii) A minimum ignition energy and critical flame radius are found in qualitative agreement with experimental observations of spark ignition.

(iii) Calculations of the effect of flame stretch on minimum ignition energy are in remarkable agreement with experimental observations of influence of turbulence on spark ignition.

(iv) The broad features of spark ignition are generated by the physical mechanisms of flame curvature and flame stretch; the
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Fig. 9. Comparison of the predicted effect of flame stretch with the measured effect of turbulent motion on spark ignition. ○ methane-air, pressure = 1 bar, ignition energy at zero stretch = 0.32 mJ, from ref. 18; ● propane-air, pressure = 0.17 bar, ignition energy at zero stretch = 3.4 mJ, from ref. 19.

Major controlling parameter is the Lewis number.

Nomenclature

- $a$: radius of the cylindrical source
- $B$: pre-exponential term in the reaction rate
- $C_p$: specific heat
- $e$: dimensional strain rate
- $E$: ignition energy
- $H$: function giving time dependence of the heat source
- $J$: monitor function
- $k$: thermal conductivity
- $L$: Lewis number
- $M$: non-dimensional reaction rate constant
- $N$: number of mesh points in space
- $Q$: heat release by chemical reaction
- $r$: non-dimensional space coordinate
- $R$: temperature rise across an adiabatic flame
- $t$: non-dimensional time
- $T$: temperature
- $u_1$: adiabatic burning velocity
- $v$: velocity
- $W$: chemical reaction rate
- $z$: dimensional space coordinate
- $Y$: reactant concentration
- $\beta$: non-dimensional activation energy
- $\delta$: adiabatic flame thickness
- $\epsilon$: non-dimensional strain rate

REFERENCES