

Chapter 6: Laminar premixed flames

Objectives

The objectives of this Chapter are:

- To develop a theory for premixed flame propagation.
- To discuss how the laminar burning velocity depends on temperature, pressure, and equivalence ratio.
- To discuss flammability limits.
- To present other features of premixed flames.

Introduction

One of the most important quantities in Combustion science is the *laminar burning velocity* (or *flame speed*), which we examine here. It refers to the velocity at which a flame propagates relative to the unburnt gas. We need this quantity to design gasoline engines, where the duration of combustion is directly related to how quickly the flame traverses the cylinder. It will also give us a general measure of the time needed to complete the chemical reactions, and hence it is useful for a variety of problems such as the rate of burning in industrial burners and in gas turbines. Finally, propagation of flames is involved in fires and accidental explosions and hence it is important to have a good grasp of the physical phenomena involved.

In Chapter 4, we studied adiabatic systems, initially at low temperature, which build-up heat slowly by the reaction and eventually ignite spontaneously. There, we saw that a competition between the rate of heat generation and the rate at which heat is lost determines whether autoignition will happen or not. In Chapter 5, we studied adiabatic vessels burning at high temperatures (the well-stirred reactor). The balance between the rate of heat generation and the rate of heat transfer out of the reactor determines the reactor temperature and its extinction.

In this Chapter, we will examine a more complex situation: the rate of heat generation balances both diffusion and convection of heat. The laminar burning velocity will be calculated by exploring the very fine balance between the terms in the energy equation of a flame.

Flame propagation

Basic description, assumptions, formulation

Consider a stationary and uniform mixture of fuel and air. Assume now a planar flame propagating in this mixture at velocity S_L , the *laminar burning velocity*. Instead of fixing the coordinate system and having the flame propagate, it is entirely equivalent to fix the flame and have the gas approaching it at speed S_L . The mixture ahead of the flame consists of unburnt reactants and the region behind the flame has the products of complete combustion and hence is at the adiabatic flame temperature T_f . Figure 6-1 shows typical temperature and species profiles across the flame. We make our usual assumptions:

- constant pressure,
- constant molecular weight, λ and c_p ,
- adiabatic flow (no heat loss),
- steady flow (no transient terms)
- one-step global chemistry (from Chapters 4 and 5),
- unity Lewis number, i.e. $\rho D = \frac{\lambda}{c_p}$.

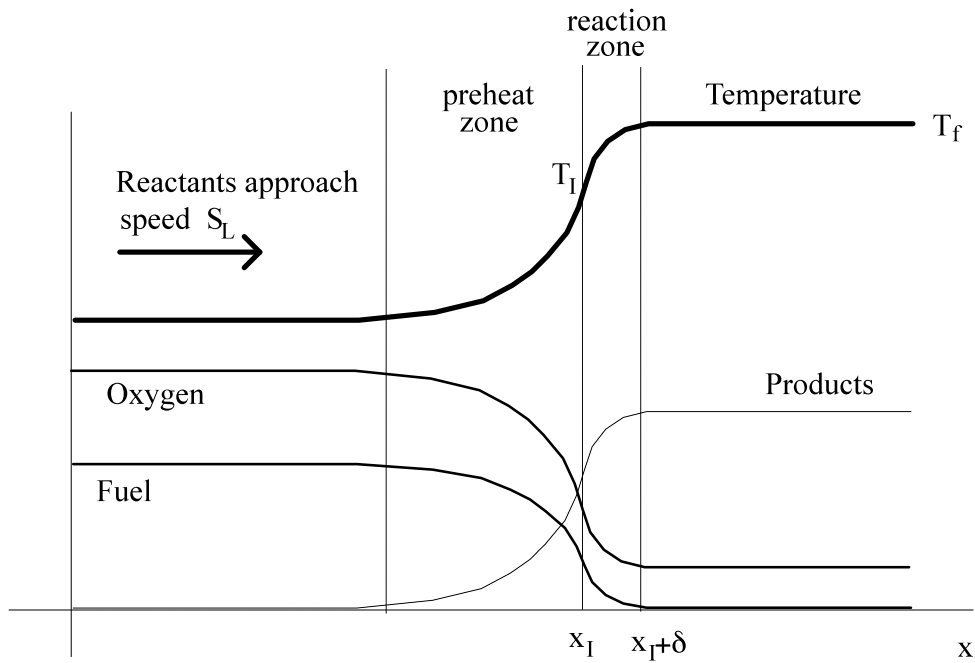


Figure 6-1. Typical profiles of temperature and species mass fractions across premixed flame. A lean flame is shown. The preheat and reaction zones are also indicated.

With these assumptions, the governing equations for species and temperature become:

$$\rho U \frac{dY_{fu}}{dx} = \frac{d}{dx} \left(\rho D \frac{dY_{fu}}{dx} \right) - \dot{w}_{fu} \quad (6.1)$$

$$\rho U \frac{dY_{ox}}{dx} = \frac{d}{dx} \left(\rho D \frac{dY_{ox}}{dx} \right) - S \dot{w}_{fu} \quad (6.2)$$

$$\rho c_p U \frac{dT}{dx} = \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + Q \dot{w}_{fu} \quad (6.3)$$

The one-step chemistry model allows the reaction rate to be written as:

$$\dot{w}_{fu} = A \frac{MW_{fu}}{MW_{fu} MW_{ox}} \rho^2 Y_{fu} Y_{ox} \exp(-E/R^0 T) \quad (6.4)$$

Note that \dot{w}_{fu} is written as positive here and hence it appears with a minus sign in the fuel conservation equation. We do this for later convenience. As we have assumed an adiabatic flame, the reactants mass fractions are related to the temperature rise (the conserved scalar concept introduced in Chapter 4 and also used in Chapter 5). The mass fractions are then given by:

$$Y_{fu} = Y_{fu,0} - c_p (T - T_0) / Q \quad (6.5)$$

$$Y_{ox} = Y_{ox,0} - S c_p (T - T_0) / Q \quad (6.6)$$

Our development will assume, strictly speaking, flames with enough oxygen to completely burn the fuel, i.e. $\phi \leq 1$, which is the situation of most practical significance. The boundary conditions at $x=0$ (unburnt mixture, subscript 0) are:

$$\begin{aligned}
Y_{fu} &= Y_{fu,0} \\
Y_{ox} &= Y_{ox,0} \\
T &= T_0 \\
d/dx &= 0 \text{ for all quantities}
\end{aligned} \tag{6.7}$$

while at $x = \infty$ (fully burnt mixture, subscript 1):

$$\begin{aligned}
\frac{dT}{dx} &= \frac{dY_{fu}}{dx} = \frac{dY_{ox}}{dx} = 0 \\
T &= T_l = T_f
\end{aligned} \tag{6.8}$$

The velocity U that appears in (6.1)-(6.3) is the local fluid velocity. Mass conservation (continuity) gives:

$$\rho U = \rho_0 U_0 = \rho_1 U_1 = \rho_0 S_L = \text{constant} \tag{6.9}$$

where the definition of the laminar burning velocity as the velocity of the incoming fluid has been employed. The group $\rho_0 S_L$ is also called the *mass burning rate* ($\text{kg/m}^2/\text{s}$). Equations (6.1) and (6.2) are not independent from (6.3), if (6.5) and (6.6) are used, and hence we need not use them any more. Just the energy equation (6.3), supplemented with (6.4), (6.5), (6.6), subject to the boundary conditions (6.7) and (6.8), and the continuity equation (6.9) is sufficient. Since the density can be found from the equation of state

$$\rho = \frac{P \overline{MW}}{R^0 T} \tag{6.10}$$

our system of equations is completely closed and can be solved, e.g. numerically. The result of that calculation would give not only the spatial distributions of temperature, velocity, and species, but also the burning velocity S_L . In essence, our system of equations has a solution that obeys the enforced boundary conditions only for a particular value of S_L , which then becomes part of the outcome of the calculation procedure. (This is because we have more boundary conditions than necessary.)

We would also like to obtain an analytical solution, so that the physics of flame propagation is better understood. Hence, below we perform a simplification to the energy governing equation that allows a closed-form expression for S_L , which is the main target of the calculation.

Simplification: energy balances across flame

Detailed analyses and experimental data have indicated that the flame can be divided into two zones: the *preheat zone* and the *reaction zone*. In the preheat zone, the rate of the reaction is negligible because the temperature is too low. This is consistent with the insight into the w_{fu} - T relationship developed in Chapters 4 and 5 (e.g. Fig. 5-2). Hence, the only terms from the energy equation active in the preheat zone is the convection and the diffusion terms. In contrast, in the reaction zone, the reaction rate is high and balances the diffusion. There, the convection term is low because, essentially, the temperature does not change very much (but the temperature profile has significant curvature to make the diffusion term high).

Combustion occurs only in the reaction zone and the heat generated there is diffused (by conduction) to the unburnt mixture through the preheat zone. Employing this simplification, we can continue our analysis for the two zones separately.

Preheat zone structure

The preheat zone extends from $x=0$ to the “ignition point” at $x=x_I$. What we mean by “ignition point” is that the reaction rate is zero for $x < x_I$, but becomes significant for $x > x_I$. The energy equation, neglecting the chemical source term, becomes:

$$\rho_0 S_L c_p \frac{dT}{dx} = \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) \quad (6.11)$$

with boundary conditions $T=T_0$ and $dT/dx=0$ at $x=0$. We have used the continuity equation (6.9). Integration of (6.11) yields

$$\rho_0 S_L c_p (T_I - T_0) = \lambda \left[\frac{dT}{dx} \right]_{x=0}^{x=x_I} \Leftrightarrow \rho_0 S_L c_p (T_I - T_0) = \lambda \left(\frac{dT}{dx} \right)_{x=x_I} \quad (6.12)$$

This equation relates the temperature at the “ignition” point to the temperature gradient there. It is an intermediate result that we will use later. We now turn our attention to the reaction zone. The following analysis will provide a second expression for the gradient at x_I .

Reaction zone structure

The reaction zone has a length δ and extends from the “ignition” point $x=x_I$ to $x=x_I+\delta$. The energy equation, neglecting convection, becomes:

$$\lambda \frac{d^2 T}{dx^2} + Q w_{fu} = 0 \quad (6.13)$$

(we now enforced the assumption of constant conductivity λ). The boundary conditions are $T=T_f$ and $dT/dx=0$ at $x=x_I+\delta$. First, we notice that

$$\frac{d}{dx} \left(\frac{dT}{dx} \right)^2 = 2 \left(\frac{dT}{dx} \right) \frac{d^2 T}{dx^2}$$

and, second, we multiply Eq. (6.13) by $2 (dT/dx)$. Then we obtain:

$$2 \left(\frac{dT}{dx} \right) \frac{d^2 T}{dx^2} = -2 \frac{Q}{\lambda} w_{fu} \left(\frac{dT}{dx} \right) \Leftrightarrow \frac{d}{dx} \left(\frac{dT}{dx} \right)^2 = -2 \frac{Q}{\lambda} w_{fu} \left(\frac{dT}{dx} \right)$$

which can be integrated to give:

$$\begin{aligned} \left[\left(\frac{dT}{dx} \right)^2 \right]_{x=x_I}^{x=x_I+\delta} &= -2 \frac{Q}{\lambda} \int_{T_I}^{T_f} w_{fu} dT \\ \Leftrightarrow 0 - \left(\frac{dT}{dx} \right)_{x=x_I}^2 &= -2 \frac{Q}{\lambda} RR \Leftrightarrow \left(\frac{dT}{dx} \right)_{x=x_I} = \sqrt{2 \frac{Q}{\lambda} RR} \end{aligned} \quad (6.14)$$

where RR is a temperature-integrated reaction rate and given by

$$RR = \int_{T_l}^{T_f} \dot{w}_{fu} dT \quad (6.15)$$

The last equality in Eq. (6.14) relates the slope at x_l with the reaction integral; the slope was related to the burning velocity through Eq. (6.12). We will calculate RR later.

Connecting the two regions: match the slopes

By matching the slopes at $x = x_l$, we obtain that:

$$\rho_0 S_L c_p (T_l - T_0) = \sqrt{2\lambda Q} RR \quad (6.16)$$

Now, we know that the reaction rate will be significant at high temperatures and so, with little error, we may assume that $T_l \approx T_f$, at least as far as the LHS of (6.16) goes. Using

$$T_f = Y_{fu,0} Q / c_p + T_0, \quad (6.17)$$

(e.g. Chapter 4, Eq. 4.7), and solving Eq. (6.17) for Q , we can substitute in Eq. (6.16) and get:

$$S_L = \sqrt{2 \left(\frac{\lambda}{\rho_0 c_p} \right) \frac{1}{\rho_0 Y_{fu,0}} \frac{RR}{(T_f - T_0)}} \quad (6.18)$$

This equation is our first important intermediate result and relates the laminar burning velocity to the mixture diffusivity ($\lambda/\rho_0 c_p$) and the reaction rate. It shows that S_L depends with equal measure on the chemistry and the diffusion processes. This justifies mathematically our physical description discussed previously. Note that it would be wrong to conclude from Eq. (6.18) that S_L increases with a reduction in fuel mass fraction or an increase in flame temperature, as the integrated reaction rate (Eq. 6.15) also depends on the fuel mass fraction and the temperature. Hence although (6.18) contains a lot of the physics, it is not straightforward to explore and understand the trends. It is instructive to go one more step and calculate approximately the reaction rate integral RR , so that a few more details on the dependences of the laminar burning velocity are revealed. We do this below.

The reaction rate integral

Here, we evaluate the reaction rate integral, Eq. (6.15), so that Eq. (6.18) can be further explored. We now use the insight that the reaction rate will be substantial only close to T_f . Hence T_l will be close to T_f , but not identical, as far as the reaction rate evaluation is concerned. The algebra is involved, but the technique shown here is very important in combustion analyses. Using Eq. (6.4):

$$\begin{aligned} RR &= \int_{T_l}^{T_f} \dot{w}_{fu} dT = \int_{T_l}^{T_f} A \frac{MW_{fu}}{MW_{fu} MW_{ox}} \rho^2 Y_{fu} Y_{ox} \exp\left(-\frac{E}{R^0 T}\right) dT \\ &\approx C \rho_1^2 \int_{T_l}^{T_f} Y_{fu} Y_{ox} \exp\left(-\frac{E}{R^0 T}\right) dT \end{aligned} \quad (6.19)$$

with ρ_l being the density of the burnt gas (i.e. at T_f). We took the density outside the integral because it does not change much from T_l to T_f . We now write the local temperature as $T = T_f - \Delta T$. This gives for the exponential:

$$\begin{aligned}\exp\left(-\frac{E}{R^0 T}\right) &= \exp\left[-\frac{E}{R^0 (T_f - \Delta T)}\right] \\ &= \exp\left[-\frac{E}{R^0 T_f (1 - \Delta T/T_f)}\right] = \exp\left[-\frac{E}{R^0 T_f} \left(1 + \frac{\Delta T}{T_f} + \dots\right)\right] \\ &\approx \exp\left(-\frac{E}{R^0 T_f}\right) \exp\left[-\frac{E}{R^0 T_f^2} (T_f - T)\right]\end{aligned}\quad (6.20)$$

This expansion is called “high activation energy expansion”. It is valid because the activation temperature is high compared to T_f , which then allows the approximation that most of the reaction occurs close to T_f . For the mass fractions now, Eqs. (6.5) and (6.6) become:

$$Y_{fu} = Y_{fu,0} - c_p (T - T_0)/Q = Y_{fu,0} - c_p (T_f - T_0)/Q + c_p (T_f - T)/Q = c_p (T_f - T)/Q \quad (6.21)$$

(through 6.17 which relates $Y_{fu,0}$ and T_f). Similarly,

$$Y_{ox} = Y_{ox,0} - SY_{fu,0} + Sc_p (T_f - T)/Q \quad (6.22)$$

Using (6.20)-(6.22), the integral in Eq. (6.19) becomes

$$\begin{aligned}&\int_{T_i}^{T_f} Y_{fu} Y_{ox} \exp\left(-\frac{E}{R^0 T}\right) dT = \\ &= \exp\left(-\frac{E}{R^0 T_f}\right) \int_{T_i}^{T_f} \left[\frac{c_p (T_f - T)}{Q}\right] \left[Y_{ox,0} - SY_{fu,0} + S\frac{c_p (T_f - T)}{Q}\right] \exp\left[-\frac{E}{R^0 T_f^2} (T_f - T)\right] dT\end{aligned}\quad (6.23)$$

To evaluate this integral easier, we now define the non-dimensional number, called the *Zel'dovich number*:

$$\beta = \frac{E}{R^0 T_f^2} (T_f - T) \quad (6.24)$$

So:

$$\begin{aligned}dT &= -\frac{R^0 T_f^2}{E} d\beta \\ \left[\frac{c_p (T_f - T)}{Q}\right] &= \frac{c_p}{Q} \frac{R^0 T_f^2}{E} \beta \\ \left[Y_{ox,0} - SY_{fu,0} + S\frac{c_p (T_f - T)}{Q}\right] &= Y_{ox,0} - SY_{fu,0} + S\frac{c_p}{Q} \frac{R^0 T_f^2}{E} \beta\end{aligned}$$

The presentation is simplified if we concentrate on stoichiometric flames, which implies that $Y_{ox,0} = SY_{fu,0}$. Hence, in terms of β , the reaction rate integral becomes:

$$\begin{aligned}
 RR &= C \rho_1^2 \int_{T_i}^{T_f} Y_{fu} Y_{ox} \exp\left(-\frac{E}{R^0 T}\right) dT \\
 &= C \rho_1^2 \left(S \frac{c_p}{Q}\right)^2 \left(\frac{R^0 T_f^2}{E}\right)^3 \exp\left(-\frac{E}{R^0 T_f}\right) \int_{\beta_i}^0 \beta^2 \exp(-\beta) d\beta
 \end{aligned} \tag{6.25}$$

there is a typo
the limits should be 0 to β_i

But $\beta_i \gg 1$ because the activation energy is high, which makes the integral in the RHS of Eq. (6.25) equal to 2 (as can be seen by integrating $\int_{\beta_i}^0 \beta^2 \exp(-\beta) d\beta$ by parts). Hence our result for the integrated reaction rate is

$$RR = C \rho_1^2 \left(S \frac{c_p}{Q}\right)^2 \left(\frac{R^0 T_f^2}{E}\right)^3 \exp\left(-\frac{E}{R^0 T_f}\right) \tag{6.26}$$

Final result for laminar burning velocity

Substituting in (6.18), and employing (6.17) solved for Q once more, our expression for the flame speed becomes:

$$S_L \approx \sqrt{2A \frac{MW_{fu}}{MW_{fu} MW_{ox}} \left(\frac{\lambda}{\rho_0 c_p}\right) \frac{\rho_1^2}{\rho_0} \frac{Y_{fu,0}}{(T_f - T_0)^3} \left(\frac{R^0 T_f^2}{E}\right)^3 \exp\left(-\frac{E}{R^0 T_f}\right)} \tag{6.27}$$

This is our final result concerning the laminar burning velocity. Equation (6.27) contains all the trends we are interested in. It was derived for stoichiometric flames, but the corresponding result for flames of any stoichiometry is not very different. The important point is that for all equivalence ratios, S_L depends on:

- the thermal diffusivity $\lambda / \rho_0 c_p$;
- the pre-exponential factor A ;
- the exponential term $\exp(-E / R^0 T_f)$.

To bring out explicitly the third dependence was the reason we performed all this lengthy development (high activation energy expansion, Zel'dovich number) to go from Eq. (6.18) to (6.27).

The laminar burning velocity: trends

Effect of fuel chemistry

This is evidenced by the pre-exponential factor A . The faster the chemistry, the faster the S_L . Hydrogen has a fast chemistry and hence hydrogen flames are much faster than hydrocarbon flames.

Effect of initial temperature

As T_0 increases, T_f increases and hence the laminar burning velocity increases through the exponential term in Eq. (6.27). Experiment shows that for most fuels, S_L grows approximately as T_0^2 , at least for a small range above room temperature (see Ex. 6-1).

Effect of mixture strength

As the mixture moves away from stoichiometry, T_f decreases and hence the flame speed decreases. Flame propagation becomes impossible for very lean or very rich mixtures (see later)

because the chemistry becomes too slow. (However, the flammability limit is a chemical effect not captured by our simple theory.)

Effect of pressure

Our model predicts that the burning velocity is independent of pressure, as the effect of pressure, through the densities in Eq. 6.27, cancels out. However, experiment shows that S_L decreases as $P^{-1/2}$. This discrepancy is due to our chemistry model (Eq. 6.4) that predicts an overall second-order reaction.

These trends are shown in more detail in Figs. 6-2 and 6-3. In general, experiment shows that all hydrocarbon fuels have approximately the same laminar burning velocity, with the exception of acetylene (C_2H_2) that is significantly faster. Hydrogen has a very high flame speed, partly due to the fast chemistry and partly due to the very high diffusion coefficient of the light hydrogen molecules. The experiment also shows that S_L peaks at ϕ slightly richer than unity, which is due to the lower heat capacity of the products of rich combustion that allows T_f to be higher there than at $\phi=1$. All in all, our theory reproduces the very important observation that the flame speed is very sensitive to flame temperature.

Flame thickness and reaction time

From the present analysis, the *flame thickness* d_L can also be estimated. As the reaction zone is very small compared to the preheat zone, the total thickness of the flame may be taken as equal to the thickness of the preheat zone. The latter can be related to the gradient of the temperature. Starting from Eq. (6.12), we get

$$\begin{aligned} \rho_0 S_L c_p (T_f - T_0) &= \lambda \left(\frac{dT}{dx} \right)_{x=x_f} \Leftrightarrow \rho_0 S_L c_p (T_f - T_0) = \lambda \frac{T_f - T_0}{d_L} \\ \Leftrightarrow d_L &= \frac{\lambda / \rho_0 c_p}{S_L} \end{aligned} \quad (6.28)$$

We may subsequently define a *chemical time* as the time taken for the reactants to go through the flame, which is

$$\tau_{chem} = \frac{d_L}{S_L} = \frac{\lambda / \rho_0 c_p}{S_L^2} \quad (6.29)$$

Definitions (6.28) and (6.29) are very useful because they allow a simple evaluation of the flame thickness and an estimate of the time needed to complete the reactions using the laminar burning velocity, which is a quantity that can be measured in an experiment relatively easily. The laminar burning velocity encompasses the rate of reaction and hence using τ_{chem} in other problems is reasonable. For example, an often-used *crude* criterion for burner stability is that the residence time should not be much less than τ_{chem} (to within a constant). Therefore flames with long τ_{chem} will be extinguished easier than flames with short τ_{chem} .

Flammability limits, quenching, spark-ignition

Lean and rich flammability limits

As we have just seen, if the flame temperature drops, the laminar burning velocity will drop due to the Arrhenius term. We have additional chemical effects if the temperature becomes too low. Below about 1500K, the chain-branching reactions that produce the radicals necessary to achieve

combustion are slow and the chain-terminating reactions dominate. This means that self-sustaining combustion becomes impossible. At very lean mixtures therefore we cannot expect flame propagation. For very rich combustion, the chemistry has additional complications in that the deficient reactant (oxygen) simply is not enough to “trigger” the chain-reactions. Hence, there is a lean and a rich limit for flame propagation, which are called *flammability limits*.

Knowledge of the flammability limits is obtained through experiment and extensive tabulated values exist (e.g. in Glassman). They are reported usually in terms of % by vol. of fuel in the mixture or in terms of the equivalence ratio. We have successful flame propagation only between the two limits.

Implications for practice

The flammability limits are very important for safety and for the proper design of combustion equipment. In industry, accidental releases of fuel vapours are not dangerous only if sufficient ventilation makes the fuel-air mixture well below the lean limit. In gasoline engines, the lean and rich limits guide the fuel preparation and the engine design. Working with lean mixtures is advantageous from a pollution point of view (low flame temperature implies low potential for NO generation; Chapter 2), but the flame may become too slow (Eq. 6.27) and hence prone to extinction.

Quenching distance

We will not go into the details of the theory here, but we state that a flame cannot propagate inside a tube with very small diameter, if the walls of the tube are kept at a low temperature. The reason is that for flame propagation, the heat generated must be allowed to diffuse towards the reactants. If heat is removed by other means (e.g. by conduction to the wall), then the flame propagation mechanism fails. The minimum pipe diameter that allows flame propagation is called the *quenching distance*. It is roughly equal to about $2d_L$.

Spark ignition

The same concept applies to successful *ignition* of flame. Spark ignition is the most common way to start a flame in practical devices. To initiate propagation, we must create a volume of hot gases of sufficient size, such that the heat transferred to the cold reactants is sufficient to raise their temperature to the “ignition” temperature (e.g. Eq. 6.12). From then on, a flame will begin to propagate. This physical intuition is summarily expressed by the following criterion for a successful spark: “A spark will be successful if it creates a region of hot gases of size roughly equal to the laminar flame thickness d_L ”. The first hot gases created by a spark are also called the *ignition kernel*.

Hence it is more difficult to ignite lean mixtures (large d_L ; see Eq. 6.26) than stoichiometric mixtures. This is the most serious problem encountered in “lean-burn” gasoline engines. Despite their thermodynamic and environmental advantages, they have not found yet widespread use because the flame is difficult to initiate. Manipulating the mixture so that it is stoichiometric close to the spark and lean elsewhere is the topic of significant effort (and expenditure!) by automotive companies.

Experimental data for burning velocities

We give below some experiment data for laminar burning velocities for hydrogen and various hydrocarbons as a function of equivalence ratio, pressure, and initial temperature. These experiments were done very carefully in order to produce steady, planar flames, but they are very difficult.

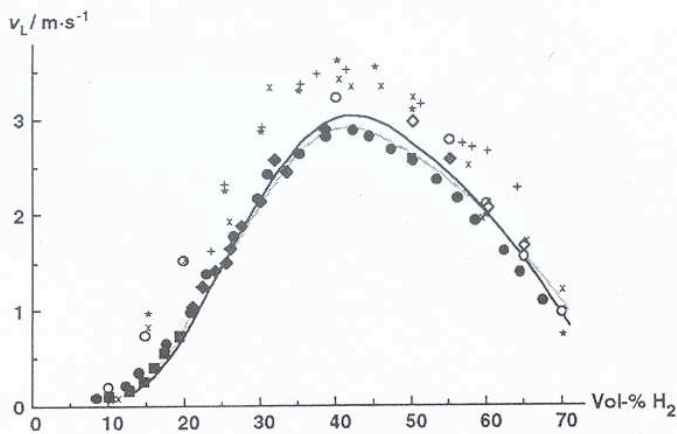


Fig. 8.10. Flame velocity in H_2 -air mixtures as function of the unburnt gas composition (Paul and Warnatz 1998) calculated with two different transport models (grey and black lines) in comparison to experiments (points), $p = 1 \text{ bar}$, $T_u = 298 \text{ K}$

(a)

Figure 6-2. Experimental data for (a) hydrogen and (b) methane laminar burning velocities. Hydrogen flames are much faster than hydrocarbon flames; S_L (V_L in the figure) decreases with pressure; S_L increases with unburnt temperature T_0 (T_u in the figure). From the book by Dibble, Mass & Warnatz, “Combustion”, Springer-Verlag, 1996.

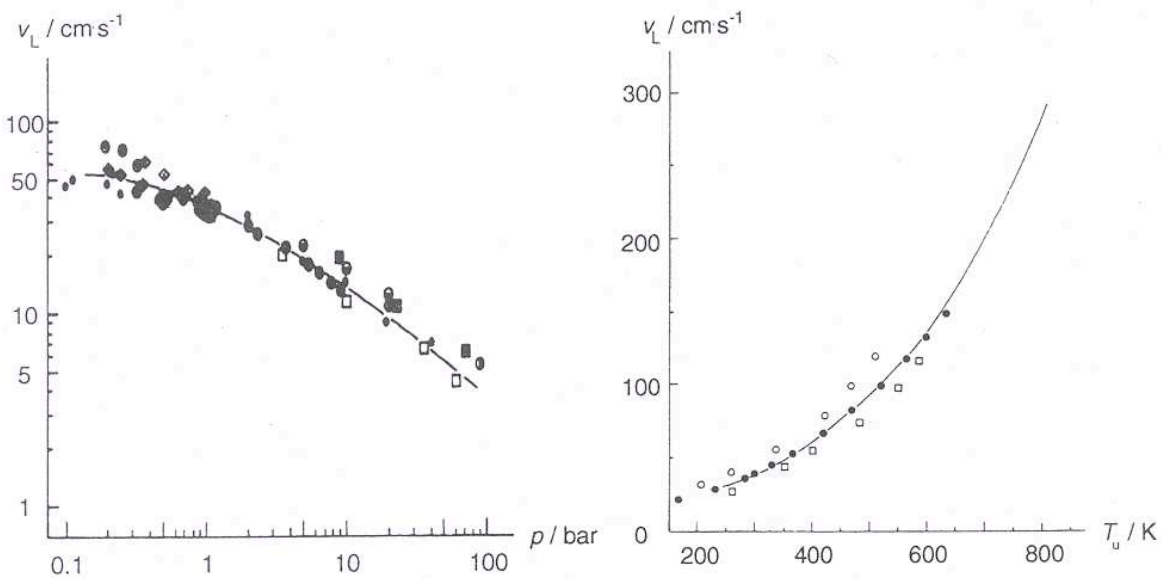


Fig. 8.11. Pressure dependence of v_L for $T_u = 298 \text{ K}$ (left) and temperature dependence of v_L for $p = 1 \text{ bar}$ (right) in stoichiometric CH_4 -air mixtures (Warnatz 1988)

(b)

Figure 6-2. Continued.

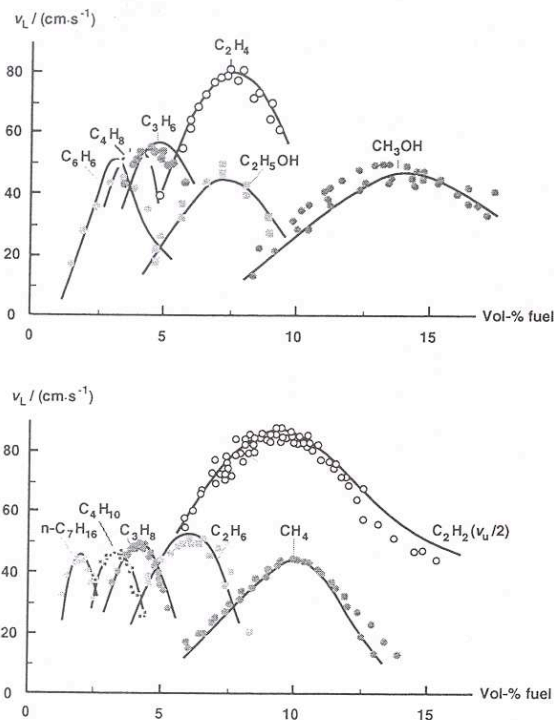


Fig. 8.12. Dependence of v_L on the mixture composition (at $p = 1$ bar, $T_u = 298$ K) for different fuel-air mixtures (Warnatz 1993)

Figure 6-3. Experimental data for laminar burning velocities for many hydrocarbons. If the data were reported with the equivalence ratio as the x-axis, the velocity would peak for all fuels at around $\phi=1$. From the book by Dibble, Mass & Warnatz, “Combustion”, Springer-Verlag, 1996.

Summary

- A premixed flame is divided into a reaction zone and a preheat zone.
- The laminar burning velocity has been calculated based on a simplified model of flame structure.
- The theory developed is approximate, but contains all the important trends.
- The laminar burning velocity peaks around stoichiometry and decreases towards lean and rich mixtures.
- The laminar burning velocity allows estimates of the flame thickness and the reaction time.
- The flammability limits denote the range of equivalence ratio where flame propagation is possible.
- To initiate a flame by a spark, the ignition kernel should have size roughly equal to the flame thickness.

Suggested reading

Turns:

Ch. 8 (253-269; 274-283; 289-294). A slightly different formulation for the reaction rate integral is given in this book. Good on the physical phenomena involved.

Glassman:

Ch. 4 (p 119; pp. 123-132; 147-155; Figs. 21, 22, 23; pp. 162-163). Closest to our analysis.

Spalding:

Ch. 18. Same formulation as in Turns. Ch. 19 describes spark ignition in detail.

Worked examples

Example 6-1. The experimental data for stoichiometric methane-air flames with reactants at $T_0=298\text{K}$ and $P=1\text{bar}$ give that $S_L=0.4\text{m/s}$. You may take a mid-range value of $c_p=1.35\text{kJ/kgK}$ and $E/R^0=20000\text{K}$. Estimate: (i) the adiabatic flame temperature; (ii) the pre-exponential factor; (iii) the flame thickness; (iv) the chemical timescale; and (v) the flame speed at $T_0=600\text{K}$.

(i) We use the relationship between initial fuel mass fraction and final temperature, $T_f = Y_{fu,0}Q/c_p + T_0$. For methane-air mixture at $\phi=1$ and writing the combustion equation, we get that $Y_{fu,0}=0.0552$ and $Y_{ox,0}=0.2201$. With $c_p=1.35\text{kJ/kgK}$ and $T_0=298\text{K}$, we get that $T_f=2341\text{K}$.


(ii) We now employ Eq. (6.27):

$$\begin{aligned}
 S_L &= \sqrt{2A \frac{MW_{fu}}{MW_{fu} MW_{ox}} \left(\frac{\lambda}{\rho_0 c_p} \right) \frac{\rho_1^2}{\rho_0} \frac{Y_{fu,0}}{(T_f - T_0)^3} \left(\frac{R^0 T_f^2}{E} \right)^3 \exp\left(-\frac{E}{R^0 T_f}\right)} \Leftrightarrow \\
 &\Leftrightarrow S_L = \sqrt{2A \frac{MW_{fu}}{MW_{fu} MW_{ox}} \left(\frac{\lambda}{c_p} \right) \left(\frac{T_0}{T_f} \right)^2 \frac{Y_{fu,0}}{(T_f - T_0)^3} \left(\frac{R^0 T_f^2}{E} \right)^3 \exp\left(-\frac{E}{R^0 T_f}\right)} \\
 &\Leftrightarrow S_L^2 = A \frac{2MW_{fu}}{MW_{fu} MW_{ox}} \left(\frac{\lambda}{c_p} \right) \left(\frac{T_0}{T_f} \right)^2 \frac{Y_{fu,0}}{(T_f - T_0)^3} \left(\frac{R^0 T_f^2}{E} \right)^3 \exp\left(-\frac{E}{R^0 T_f}\right)
 \end{aligned}$$

We have assumed that the ratio of burnt to unburnt densities is given by the ratio of temperatures, which is a good approximation because the mixture molecular weight is almost the same and equal to the MW of air. From Tables, $\lambda=0.026\text{J/msK}$ (for air at 298K). Solving for A , $A=3.34 \times 10^{14} (\text{kmol m}^3)^{-1} \text{s}^{-1}$.

(iii) The flame thickness is $d_L = \frac{\lambda / \rho_0 c_p}{S_L} = 0.04 \text{ mm}$.

(iv) The chemical timescale is $\tau_{chem} = \frac{d_L}{S_L} = 0.1 \text{ ms}$.

(v) If $T_0=600\text{K}$, we get $T_f=2643\text{K}$. Evaluating the expression for S_L , we get that $S_L=1.72 \text{ m/s}$. 

Notes:

- The flame thickness may appear too small, but this is due to the definition we employed. Normally, because the temperature profile “flattens out” towards the reactants, the thickness of the preheat zone is about 3-4 times our estimate. A typical hydrocarbon flame at atmospheric conditions has a total thickness of a fraction of a millimetre.
- The “rule-of-thumb” that the flame speed increases with the square of T_0 is substantiated by the full calculation: the “T-square” dependence would give $(600/298)^2 \cdot 0.4 = 1.62 \text{ m/s}$.
- The pre-exponential factor calculated here should be thought of as a part of the whole one-step chemical model, “tuned” so as to give the right S_L . So, the pre-exponential factor A would have to be different if E/R^0 were different and if the global reaction was not taken to be as second-order. The exact choice made depends on the particular problem and is outside the scope of this course.