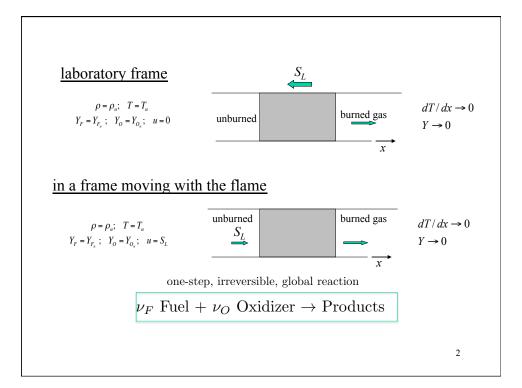
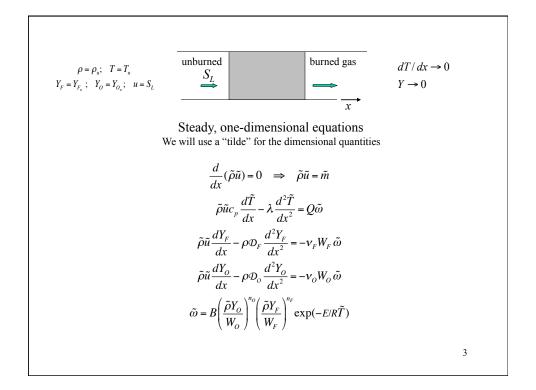


The Structure of a Planar Laminar Flame

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$$\tilde{\rho}\tilde{u} = const.$$

$$\tilde{\rho}\tilde{u}c_{p}\frac{d\tilde{T}}{dx} - \lambda \frac{d^{2}\tilde{T}}{dx^{2}} = Q\tilde{\omega}$$

$$\tilde{\rho}\tilde{u}\frac{dY_{F}}{dx} - \rho \mathcal{D}_{F}\frac{d^{2}Y_{F}}{dx^{2}} = -v_{F}W_{F}\tilde{\omega}$$
Assume the mixture is lean; this implies that the fuel is completed depleted
$$\frac{d}{dx}\left[\tilde{\rho}\tilde{u}\left(c_{p}\tilde{T} + \frac{QY_{F}}{v_{F}W_{F}}\right)\right] - \frac{d}{dx}\left[\lambda\frac{d\tilde{T}}{dx} + \frac{\rho \mathcal{D}_{F}Q}{v_{F}W_{F}}\frac{dY_{F}}{dx}\right] = 0$$
Integrating from - ∞ to + ∞ and using the BCs, yields
$$\tilde{\rho}\tilde{u}\left(c_{p}\tilde{T} + \frac{QY_{F}}{v_{F}W_{F}}\right)\right]_{-\infty}^{\infty} = 0$$
Similarly for a rich mixture. Use the equation for Y_{O} instead of that of Y_{F} and assume now that all the oxidizer is depleted.
$$\tilde{T}_{u} = \begin{cases} \tilde{T}_{u} + \frac{(Q/c_{p})Y_{F_{u}}}{v_{p}W_{p}} & \phi < 1\\ \tilde{T}_{u} + \frac{(Q/c_{p})Y_{O_{u}}}{v_{0}W_{0}} & \phi > 1 \end{cases}$$

The residual fuel/oxidizer can be computed from

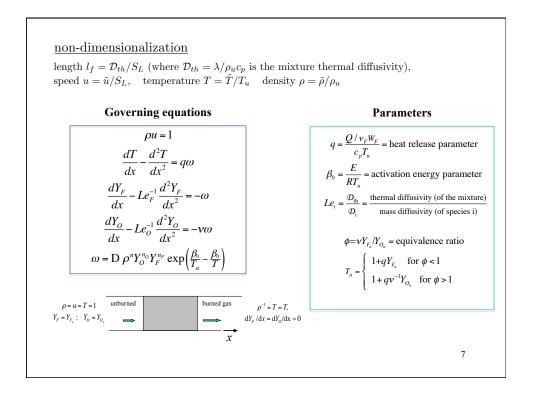
$$\tilde{\rho}\tilde{u}\frac{dY_F}{dx} - \rho\mathcal{D}_F\frac{d^2Y_F}{dx^2} = -v_FW_F\tilde{\omega}$$
$$\tilde{\rho}\tilde{u}\frac{dY_O}{dx} - \rho\mathcal{D}_O\frac{d^2Y_O}{dx^2} = -v_OW_O\tilde{\omega}$$
$$\frac{d}{dx}\left[\tilde{\rho}\tilde{u}\left(\frac{Y_O}{v_OW_O} - \frac{Y_F}{v_FW_F}\right)\right] - \frac{d}{dx}\left[\frac{\rho\mathcal{D}_O}{v_OW_O}\frac{dY_O}{dx} - \frac{\rho\mathcal{D}_F}{v_FW_F}\frac{dY_F}{dx}\right] = 0$$
Integrating from - ∞ to + ∞ and using the BCs, yields
$$Y_F = 0, \qquad Y_O = Y_{O_u}(1-\phi) \qquad \text{for } \phi < 1$$
$$Y_O = 0, \qquad Y_F = Y_{F_u}(1-\phi^{-1}) \qquad \text{for } \phi > 1$$

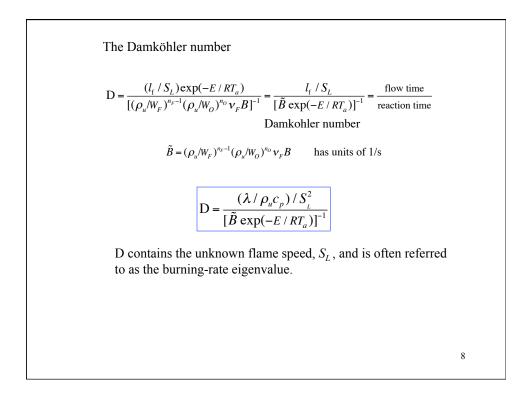
 $\tilde{\rho}\tilde{u}c_{p}\frac{d\tilde{T}}{dx} - \lambda \frac{d^{2}\tilde{T}}{dx^{2}} = Q\tilde{\omega}$ $\tilde{\rho}\tilde{u}\frac{dY_{F}}{dx} - \rho \mathcal{D}_{F}\frac{d^{2}Y_{F}}{dx^{2}} = -v_{F}W_{F}\tilde{\omega}$ $\tilde{\omega} = B\left(\frac{\tilde{\rho}Y_{O}}{W_{O}}\right)^{v_{O}}\left(\frac{\tilde{\rho}Y_{F}}{W_{F}}\right)^{v_{F}}\exp(-E/R\tilde{T})$ $\tilde{\rho}\tilde{u}\frac{dY_{O}}{dx} - \rho \mathcal{D}_{O}\frac{d^{2}Y_{O}}{dx^{2}} = -v_{O}W_{O}\tilde{\omega}$ $\tilde{\rho} = \rho_{u}; \quad \tilde{T} = T_{u}; \quad d\tilde{T}/dx = 0; \quad Y_{F} = Y_{F_{u}}; \quad Y_{O} = Y_{O_{u}}; \quad \tilde{u} = S_{L} \text{ as } x \to -\infty$ $d\tilde{T}/dx = dY_{F}/dx = dY_{O}/dx = 0 \quad \text{ as } x \to +\infty$ The problem is mathematically ill-posed because the reaction rate does not vanish at the far left (<u>the cold boundary difficulty</u>). The difficulty is due to the idealization (infinite domain) and the nature of the Arrhenius law. Can be resolved
(i) if the mixture is introduced at a finite location (i.e. a burner)

(ii) by introducing a switch-on temperature; i.e. multiply the RHS by $H(T - T_i)$. These resolutions are not needed when the asymptotic solution for large activation energy is sought.

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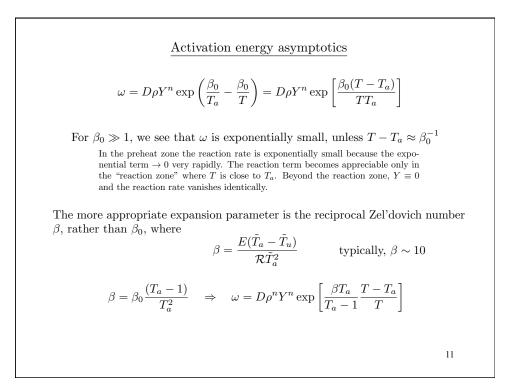
For simplicity of presentation we will consider first a mixture deficient in one component; i.e either lean (fuel deficient) of rich (oxidizer deficient), for which the excess component remains nearly unchanged¹. We thus remove all subscripts, and denote by Y the mass fraction of the deficient component. Results for the general case will be presented later.

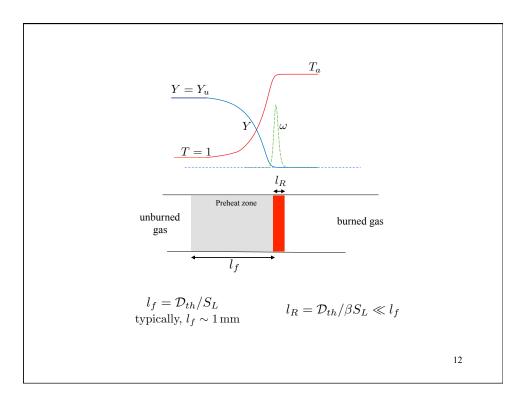
$$\frac{dT}{dx} - \frac{d^2T}{dx^2} = q\omega \qquad dT/dx = 0, \ T = 1, \ Y = Y_u \\ as \ x \to -\infty \qquad as \ x \to -\infty \qquad T = T_a, \ Y = 0 \\ \omega = D\rho^n Y^n \exp\left(\frac{\beta_0}{T_a} - \frac{\beta_0}{T}\right) \qquad as \ x \to \infty$$

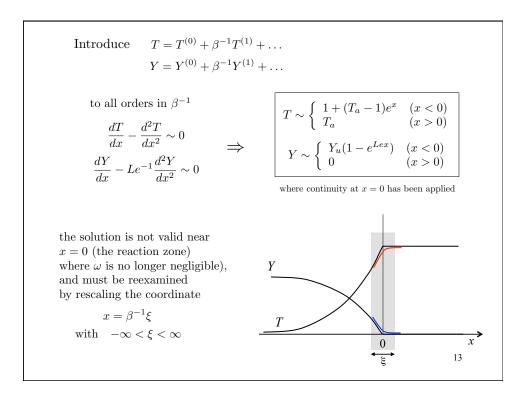
nonlinear eigenvalue problem for the determination of T, Y and D

$$Le = \frac{\mathcal{D}_{\text{th}}}{\mathcal{D}_{\text{m}}} = \frac{\text{thermal diffusivity (of the mixture)}}{\text{mass diffusivity (of deficient reactant)}} \qquad \text{in lean mixtures: } \mathcal{D}_{\text{m}} = \mathcal{D}_{\text{fuel}}$$
$$\text{in rich mixtures } \mathcal{D}_{\text{m}} = \mathcal{D}_{\text{oxidizer}}$$

¹ We are effectively considering the case $R \to P$, for which the reaction is of 10 order n, or $n_F = n$, $n_O = 0$, and $\nu_F = 1$.







Reaction zone solution introducing a stretching transformation, $x = \beta^{-1}\xi$, into the governing equations, we seek solutions of the form $T = T_a + \beta^{-1}\phi(\xi) + \cdots$ $Y = \beta^{-1}\psi(\xi) + \cdots$ with the "eigenvalue" expanded as $D = \beta^{n+1}\Lambda + \cdots$ $\beta^{-1}\frac{d\phi}{d\xi} - \frac{d^2\phi}{d\xi^2} + \cdots = q\Lambda\rho_b^n \psi^n e^{\phi/(T_a - 1)}$ $\beta^{-1}\frac{d\psi}{d\xi} - Le^{-1}\frac{d^2\psi}{d\xi^2} + \cdots = -\Lambda\rho_b^n \psi^n e^{\phi/(T_a - 1)}$ the reaction zone is a diffusive-reactive zone, with convection playing a secondary role here ρ_b is the (dimensionless) density of the burned gas = $1/T_a$ The expansion of the exponential yields $\exp\left[\frac{\beta T_a}{T_a - 1}\frac{T - T_a}{T}\right] = \exp\left[\frac{\beta}{T_a - 1}(\beta^{-1}\phi + \cdots)\right] \sim \exp\left[\phi/(T_a - 1)\right]$ 14

$$\begin{aligned} \frac{d^2\phi}{d\xi^2} &= -q\Lambda\rho_b^n \ \psi^n e^{\phi/(T_a-1)} \\ Le^{-1}\frac{d^2\psi}{d\xi^2} &= \Lambda\rho_b^n \ \psi^n e^{\phi/(T_a-1)} \\ \text{The solution for } \phi \text{ and } \psi \text{ must match } T \text{ and } Y \text{ as } \xi \to \mp \infty \\ \frac{d\phi}{d\xi} &\sim (T_a-1), \quad \frac{d\psi}{d\xi} &\sim -Y_u Le \quad \text{ as } \xi \to -\infty \\ \phi &\sim \psi &\sim 0, \quad \text{ as } \xi \to +\infty \end{aligned}$$

using
$$T \sim \begin{cases} 1+(T_a-1)e^x \ (x < 0) \\ T_a \ (x > 0) \end{cases} \qquad Y \sim \begin{cases} Y_u(1-e^{Lex}) \ (x < 0) \\ 0 \ (x > 0) \end{cases} \\ T \sim \begin{cases} T_a + \beta^{-1}(T_a-1)\xi \ \text{ as } \xi \to -\infty \\ T_a \ (x < 0) \ (x > 0) \end{cases} \end{cases} \qquad T \sim \begin{cases} T_a + \beta^{-1}(T_a-1)\xi \ \text{ as } \xi \to -\infty \\ \theta &\propto \xi \to +\infty \end{cases}$$

For n = 1

$$S_L = \sqrt{\frac{\tilde{\rho_b}}{\tilde{\rho}_u^2} \frac{2(\lambda/\tilde{c}_p)B}{\beta^2 L e^{-1}}} \ e^{-E/2\mathcal{R}\tilde{T}_a}$$

Arbitrary reaction order n

$$S_L = \sqrt{\frac{\tilde{\rho}_b^n}{\tilde{\rho}_u^2} \frac{2\Gamma(n+1)(\lambda/\tilde{c}_p)BY_u^{n-1}}{W^{n-1}\beta^{n+1}Le^{-n}}} \ e^{-E/2\mathcal{R}\tilde{T}_a}$$

Adiabatic flame temperature $\tilde{T}_a = \tilde{T}_u + (Q/c_p)Y_u$

Flame thickness (thermal) $l_f = \lambda / \tilde{\rho}_u c_p S_L$

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Recall that we have been considering here the very lean (or very rich) case; i.e., the reaction is of order n in the deficient component and is independent of the abundant reactant.

<u>Comments</u>:

- Most of the reaction occurs, in a narrow temperature interval near T_a which is on the order $\beta^{-1}l_f\equiv l_R$
- The preheat zone is the region where the temperature rises from T_u to approximately T_a . Most of this increase (more than 99%) occurs in 5 units of length, so that the actual width of the preheat zone is $\sim 5l_f$
- The analysis could be easily extended to account for temperature-dependent transport since this will only affect the preheat zone. The resulting profiles (with λ measured with respect to its value in the unburned gas) are

$$T = 1 + (T_a - 1)e^{-\int_x^0 \frac{1}{\lambda} dx'} \qquad Y = Y_u [1 - e^{-\int_x^0 \frac{1}{\lambda} dx'}]$$

The consequence on the flame speed is that λ needs to be evaluated at T_a .

• To complete the solution we note that $\rho = 1/T$ and u = T; as a result of gas expansion the density decreases and the gas speeds up. The pressure drop across the flame, calculated from the momentum equation, is

$$p \sim \begin{cases} -(1 - \frac{4}{3} \Pr)(T_a - 1)e^x & (x < 0) \\ -(T_a - 1) & (x > 0) \end{cases}$$

- It is possible to find the next correction to the burning rate eigenvalue. For n = 1 if

$$D = \beta^2 (\Lambda_0 + \beta^{-1} \Lambda_1 + \cdots)$$

one finds

$$S_L = \sqrt{\frac{\tilde{\rho}_b}{\tilde{\rho}_a^2} \frac{2(\lambda/\tilde{c}_p)B}{\beta^2 L e^{-1}}} e^{-E/2\mathcal{R}\tilde{T}_a} \left[1 + \beta^{-1} \left(1.344 - 3\frac{\tilde{T}_a - \tilde{T}_a}{\tilde{T}_a}\right)\right]$$

• The strong dependence of the Arrhenius rate, and hence of the flame speed on temperature suggests that a small temperature variation cause a significant change in speed; more precisely $O(\beta^{-1})$ changes in T_a cause O(1) changes in S_L .

• The effect of stoichiometry is found by considering a two-reactants system. For n = 2, with $n_F = n_O = 1$, the flame speed generalizes to

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$$S_L = \sqrt{\frac{\tilde{\rho}_b^2}{\tilde{\rho}_u^2}} \frac{2B(\lambda/c_p)}{\beta^2} \mathcal{S} \ e^{-E/2\mathcal{R}\tilde{T}_a}$$

where $\mathcal{S} \sim \begin{cases} Le_F \frac{\nu_F Y_{O_u}}{W_O} [(1-\phi) + 2\beta^{-1}Le_O \phi] & (\phi < 1) \\ Le_O \frac{\nu_O Y_{F_u}}{W_F} [(1-\phi^{-1}) + 2\beta^{-1}Le_F \phi^{-1}] & (\phi < 1) \end{cases}$

with $\phi = \nu Y_{Fu}/Y_{Ou}$ the equivalence ratio and $\nu = \nu_O W_o/\nu_F W_F$.

• Note that at stoichiometry ($\phi = 1$), the two expressions are identical and reduce to

$$S_{L} = \sqrt{\frac{\tilde{\rho}_{b}^{2}}{\tilde{\rho}_{u}^{2}}} \frac{4B(\lambda/c_{p})}{\beta^{3}Le_{F}^{-1}Le_{O}^{-1}} \frac{\nu_{F}Y_{Ou}}{W_{O}} e^{-E/2\mathcal{R}\tilde{T}_{a}}$$

Some observations from the derived expressions

- The adiabatic flame temperature T_a exerts the strongest influence on S_L , so that reactions with larger values of heat release Q propagate faster flames.
- The flame speed S_L increases with increasing T_u .
- The flame gets thinner when increasing Q or T_u .
- The adiabatic flame temperature peaks at stoichiometry. The dependence $S_L \sim \sqrt{Le_F Le_O}$, however, suggests that there will be a shift in the peaking of the flame speed towards the lean or rich side, depending on the fuel. For hydrogen, for example, the peaking is towards the rich side because of the the relatively low value of Le_F that is dominant under lean conditions.
- The dependence of S_L , and hence of l_f , on pressure depends on the reaction order;

$$S_L \sim \frac{\tilde{\rho_b}^{n/2}}{\tilde{\rho}_u} \sim P^{\frac{n}{2}-1} \qquad l_f = \lambda/\rho_u c_p S_L \sim P^{-\frac{n}{2}}$$

generally n < 2 and S_L decreases slightly with pressure, but it is independent of pressure for a second order reaction

The flame thickness, however, always decreases with increasing pressure

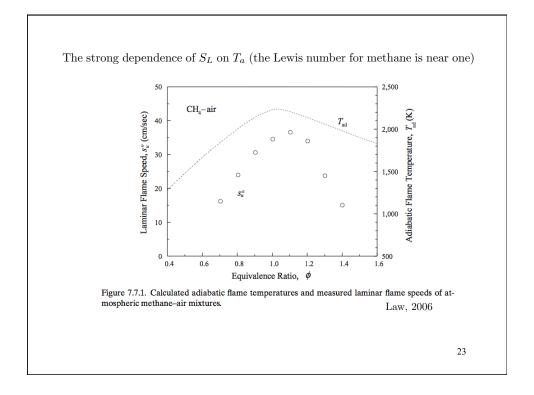
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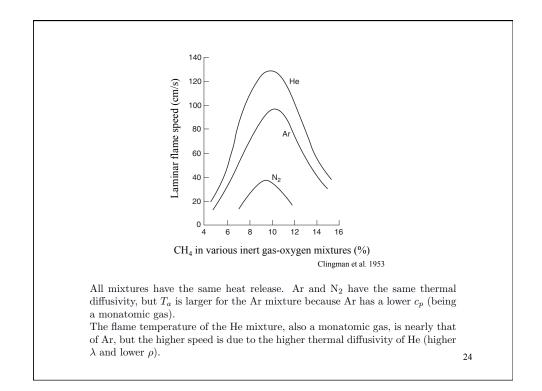
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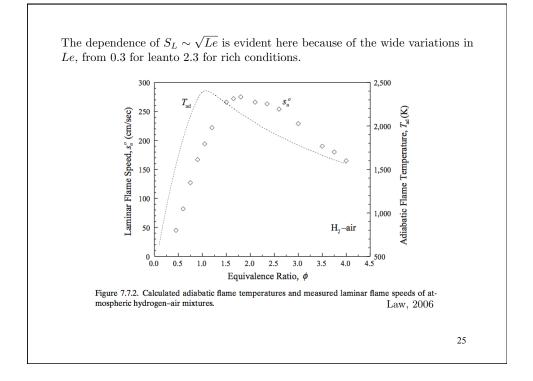
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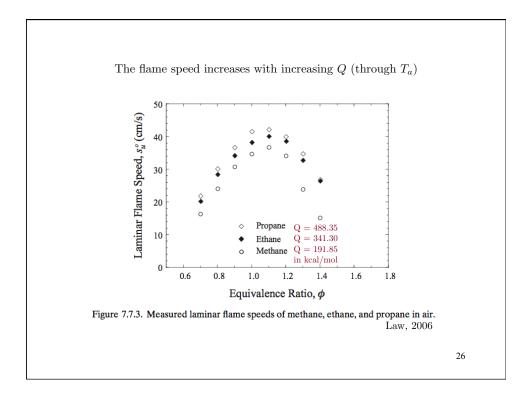
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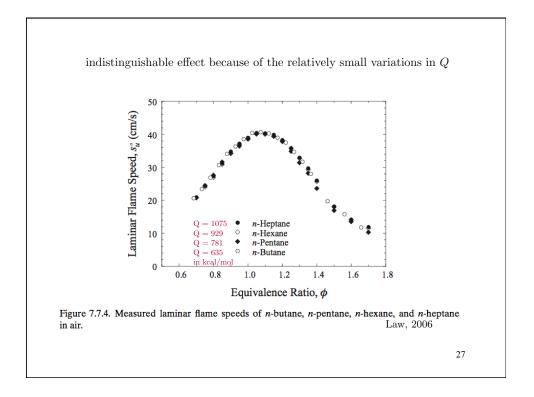
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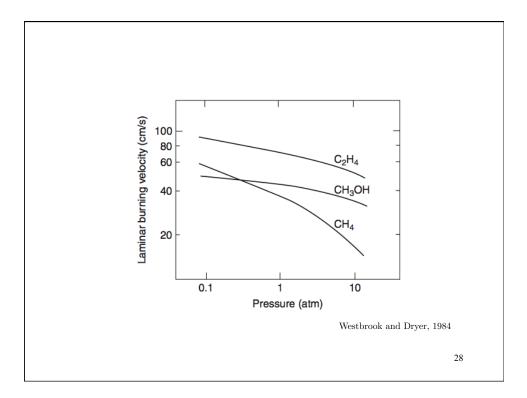












Summary and Generalization

The asymptotic treatment shows that the reaction zone, as seen from the relatively larger scale of the flame l_f , is a discontinuity across which the variables remain continuous but their derivatives jump. Furthermore, it states that the flux of reactants to the sheet (determined from the internal structure of the reaction zone) is an Arrhenius function of the flame temperature T_f .

