



Outline

USC Viterbi
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- Review of conservation equations
- Premixed flame structure & propagation rate
- Nonpremixed flames
 - Flat unstretched flames
 - Stretched flames
 - Liquid fuel droplet combustion

Conservation eqns. - energy & species

- Combined effects of unsteadiness, convection, heat conduction or mass diffusion and sources/sinks

$$\rho \left[\frac{\partial h}{\partial t} + (\vec{u} \cdot \vec{\nabla} h) \right] - \vec{\nabla} \cdot (k \vec{\nabla} T) = \dot{q}'''; \rho \left[\frac{\partial Y_i}{\partial t} + (\vec{u} \cdot \vec{\nabla} Y_i) \right] - \vec{\nabla} \cdot (\rho D \vec{\nabla} Y_i) = M_i \omega_i$$

- Special case: 1D, steady ($\partial/\partial t = 0$), constant C_p (thus $dh/dx = C_p dT/dx$) & constant k :

$$\rho u \frac{dT}{dx} - \frac{k}{C_p} \frac{d^2 T}{dx^2} = \frac{\dot{q}'''}{C_p}; \rho u \frac{dY_i}{dx} - \rho D \frac{d^2 Y_i}{dx^2} = M_i \omega_i$$

- Note if $\rho D = k/C_p$ and there is only a single reactant with heating value Q_R , then $\dot{q}''' = -Q_R M_i \omega_i$ and the equations for T and Y_i are exactly the same!
- Note also for 1D, $\rho u = \dot{m}/A = \text{constant}$
- $k/\rho C_p D$ is dimensionless, called the **Lewis number (Le)** – generally for gases $D \approx k/\rho C_p \approx \nu$, where $k/\rho C_p = \alpha = \text{thermal diffusivity}$, $\nu = \text{kinematic viscosity}$ (“viscous diffusivity”)
- $\rho \sim P/T$, $k \sim P^{0.7}$, $C_p \sim T^{0.7}$, so all 3 types of diffusivity $\sim P^{-1} T^{1.7}$

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Conservation eqns. - energy & species

- Combine energy and species equations, non-dimensionalize

$$\left[\frac{\partial Y_i}{\partial t} + (\vec{u} \cdot \vec{\nabla} Y_i) \right] - D \vec{\nabla} \cdot (\vec{\nabla} Y_i) = \frac{M_i \dot{\omega}_i}{\rho} \Rightarrow \left[\frac{\partial Y_i}{\partial t} + (\vec{u} \cdot \vec{\nabla} Y_i) \right] - \frac{\alpha}{Le} \vec{\nabla} \cdot (\vec{\nabla} Y_i) = \frac{M_i \dot{\omega}_i}{\rho}$$

$$\left[\frac{\partial T}{\partial t} + (\vec{u} \cdot \vec{\nabla} T) \right] - \frac{k}{\rho C_p} \vec{\nabla} \cdot (\vec{\nabla} T) = \dot{q}''' = -\frac{M_i \dot{\omega}_i Q_R}{\rho C_p}; \text{ Let } \tilde{T} = \frac{T - T_\infty}{Y_{i,\infty} Q_R / C_p} = \frac{T - T_\infty}{T_{ad} - T_\infty}, \tilde{Y} = \frac{Y_i}{Y_{i,\infty}}$$

$$\Rightarrow \left[\frac{\partial \tilde{T}}{\partial t} + (\vec{u} \cdot \vec{\nabla} \tilde{T}) \right] - \alpha \vec{\nabla} \cdot (\vec{\nabla} \tilde{T}) = -\frac{M_i \dot{\omega}_i}{\rho Y_{i,\infty}}; \left[\frac{\partial \tilde{Y}}{\partial t} + (\vec{u} \cdot \vec{\nabla} \tilde{Y}) \right] - \frac{\alpha}{Le} \vec{\nabla} \cdot (\vec{\nabla} \tilde{Y}) = \frac{M_i \dot{\omega}_i}{\rho Y_{i,\infty}}$$

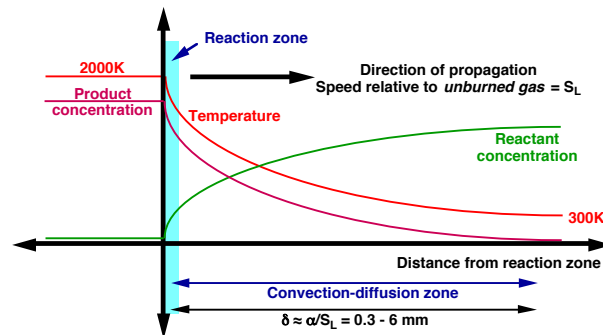
$$\text{Add species \& energy equations for } Le = 1: \left[\frac{\partial (\tilde{T} + \tilde{Y})}{\partial t} + (\vec{u} \cdot \vec{\nabla} (\tilde{T} + \tilde{Y})) \right] - \alpha \vec{\nabla} \cdot (\vec{\nabla} (\tilde{T} + \tilde{Y})) = 0$$

- For $Le = 1$, $\tilde{T} + \tilde{Y} = 1$ is constant, i.e., doesn't vary with reaction
 - Unburned gas: $\tilde{T} = 0, \tilde{Y} = 1$; burned gas: $\tilde{T} = 1, \tilde{Y} = 0$
 - If Le is not exactly 1, small deviations in Le (thus T) will have large impact on ω due to high activation energy
 - Energy equation may have heat loss in \dot{q}''' term, not present in species conservation equation, which would break the symmetry of the equations even for $Le = 1$

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Schematic of deflagration (from Lecture 1)



- Temperature increases in **convection-diffusion zone** or **preheat zone** ahead of reaction zone, even though no heat release occurs there, due to balance between convection & diffusion
- Temperature constant downstream (if adiabatic)
- Reactant concentration decreases in convection-diffusion zone, even though no chemical reaction occurs there, for the same reason

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Convection-diffusion zones

- Outside of a thin reaction zone defined to be at $x = 0$

$$\frac{dT}{dx} - \frac{k}{\rho u C_p} \frac{d^2T}{dx^2} = 0; \rho u = \frac{\dot{m}}{A} = \text{constant}; \text{2nd order O.D.E}$$

Boundary conditions **upstream** of reaction zone: $x = 0, T = T_{ad}; x \rightarrow \infty, T \rightarrow T_{\infty}$

$$\Rightarrow T(x) = T_{\infty} + (T_{ad} - T_{\infty}) e^{-x/\delta}; \delta \equiv \frac{-k}{\rho u C_p} = \frac{k}{\rho_{\infty} S_L C_p}$$

Boundary conditions **downstream** of reaction zone: $x = 0, T = T_{ad}; x \rightarrow -\infty, T \rightarrow T_{ad}$
 $\Rightarrow T(x) = T_{ad} = \text{constant}$

- Temperature profile is exponential in this **convection-diffusion zone** ($x \geq 0$); constant downstream ($x \leq 0$)
- $u = -S_L$ ($S_L > 0$) at $x = +\infty$ (flow from right to left in figure on previous page); in premixed flames, S_L is called the **burning velocity**
- δ has units of length: **flame thickness** in premixed flames
- Within reaction zone – temperature does not increase despite heat release – temperature acts to change slope of temperature profile, not temperature itself

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Reaction-diffusion zones

- In limit of infinitely thin reaction zone, T does not change but dT/dx does; integrating across reaction zone

$$\int_{0-}^{0+} u \frac{dT}{dx} dx - \int_{0-}^{0+} \alpha \frac{d^2T}{dx^2} dx = \int_{0-}^{0+} \frac{\dot{q}'''}{\rho C_p} dx \Rightarrow uT \Big|_{0-}^{0+} - \alpha \frac{dT}{dx} \Big|_{0-}^{0+} = \int_{0-}^{0+} \frac{\dot{q}'''}{\rho C_p} dx$$

$$\Rightarrow -\left(\frac{dT}{dx} \Big|_{x=0+} - \frac{dT}{dx} \Big|_{x=0-} \right) = \int_{0-}^{0+} \frac{\dot{q}'''}{k} dx = \int_{0-}^{0+} \frac{\dot{q}''' A dx}{kA} = \int_{0-}^{0+} \frac{\dot{q}''' dV}{kA}$$

$$\Rightarrow \left(\frac{dT}{dx} \Big|_{x=0+} - \frac{dT}{dx} \Big|_{x=0-} \right) = -\frac{\dot{m} Q_R}{kA} = -\frac{\rho_\infty S_L A C_p (T_{ad} - T_\infty)}{kA} = -\frac{(T_{ad} - T_\infty)}{\delta}$$

- Note that this can also be seen from temperature profile:

$$\left. \begin{aligned} T(x) &= T_\infty + (T_{ad} - T_\infty) e^{-x/\delta} \quad (x \geq 0) \\ T(x) &= T_{ad} = \text{constant} \quad (x \leq 0) \end{aligned} \right\} \Rightarrow \left(\frac{dT}{dx} \Big|_{x=0+} - \frac{dT}{dx} \Big|_{x=0-} \right) = -\frac{(T_{ad} - T_\infty)}{\delta}$$

- Thus, **change in slope of temperature profile is a measure of the total amount of reaction** – but only when the reaction zone is thin enough that convection term can be neglected compared to diffusion term

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Deflagrations - burning velocity

- Recall $P_2 \approx P_1$ for deflagrations – but if $P_2 = P_1$, what moves the gas?
 - Mass conservation, 1D: $\dot{m} / A = \rho_1 u_1 = \rho_2 u_2$; $u_1 = S_L$
 - Momentum conservation, 1D: $P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2$
 - Ideal gas: $P_1 = \rho_1 R T_1$; $P_2 = \rho_2 R T_2$
 - Combine; estimate using typical values for stoich. hydrocarbon-air:

$$\frac{P_2 - P_1}{P_1} \approx \frac{S_L^2}{R T_1} \left(1 - \frac{T_2}{T_1} \right) = \frac{(0.4 \text{ m/s})^2}{\left(287 \frac{\text{J}}{\text{kgK}} \right) (298 \text{ K})} \left(1 - \frac{2200 \text{ K}}{300 \text{ K}} \right) = -1.18 \times 10^{-5}$$

- Thus, the dynamic pressure change across the deflagration $P_2 - P_1$ is very small compared to the thermodynamic pressure P_1
- How fast will the flame propagate? Simplest estimate based on the hypothesis that
 - Rate of heat conducted from hot gas to cold gas (i) =
 - Rate at which enthalpy is convected through flame front (ii) =
 - Rate at which thermal enthalpy is produced by chemical reaction (iii)

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Deflagrations - burning velocity

- Estimate of i
Conduction heat transfer rate = $-kA(\Delta T/\delta)$
 k = gas thermal conductivity, A = cross-sectional area of flame
 ΔT = temperature rise across front = $T_{\text{products}} - T_{\text{reactants}}$
 δ = thickness of front (unknown at this point)
- Estimate of ii
Enthalpy flux through front = (mass flux) $\times C_p \times \Delta T$
Mass flux = $\rho u A$ (ρ = density of reactants = ρ_∞ , u = velocity = S_L)
Enthalpy flux = $\rho_\infty C_p S_L A \Delta T$
- Estimate of iii
Heat generated by reaction = $Q_R \times (d[\text{fuel}]/dt) \times M_{\text{fuel}} \times \text{Volume}$
Volume = $A\delta$
 $Q_R = C_p \Delta T / f$
$$f = \frac{\text{Fuel mass}}{\text{Total mass}} = \frac{(\text{Mass fuel} / \text{volume})}{(\text{Mass total} / \text{volume})}$$

$$= \frac{(\text{Moles fuel} / \text{volume})(\text{mass fuel} / \text{moles fuel})}{(\text{Mass total} / \text{volume})} = \frac{[F]_\infty M_{\text{fuel}}}{\rho_\infty}$$

$[F]_\infty$ = fuel concentration in the cold reactants

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Deflagrations - burning velocity

- Combine (i) and (ii)
 - $\delta = k/\rho C_p S_L = \alpha/S_L$ (δ = flame thickness) (same as Lecture 7)
 - Recall $\alpha = k/\rho C_p$ = thermal diffusivity (units length²/time)
 - For air at 300K & 1 atm, $\alpha \approx 0.2$ cm²/s
 - For gases $\alpha \approx \nu$ (ν = kinematic viscosity)
 - For gases $\alpha \sim P^{-1}T^{1.7}$ since $k \sim P^0T^{.7}$, $\rho \sim P^1T^{-1}$, $C_p \sim P^0T^0$
 - For typical stoichiometric hydrocarbon-air flame, $S_L \approx 40$ cm/s, thus $\delta \approx \alpha/S_L \approx 0.005$ cm (!) (Actually when properties are temperature-averaged, $\delta \approx 4\alpha/S_L \approx 0.02$ cm - still small!)
- Combine (ii) and (iii)
 - $S_L = (\alpha\omega)^{1/2}$
 - ω = overall reaction rate = $(d[\text{fuel}]/dt)/[\text{fuel}]_\infty$ (units 1/s)
 - With $S_L \approx 40$ cm/s, $\alpha \approx 0.2$ cm²/s, $\omega \approx 1600$ s⁻¹
 - $1/\omega$ = characteristic reaction time = 625 microseconds
- Heat release rate per unit volume = (enthalpy flux) / (volume)
 - = $(\rho C_p S_L A \Delta T)/(A\delta) = \rho C_p S_L/k(k\Delta T)/\delta = (k\Delta T)/\delta^2$
 - = $(0.07 \text{ W/mK})(1900\text{K})/(0.0002 \text{ m})^2 = 3 \times 10^9 \text{ W/m}^3$!!!
- Moral: flames are thin, fast and generate a lot of heat!

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Deflagrations - burning velocity

- How does S_L vary with pressure?

$$\frac{d[A]}{dt} = -k_f [A]^{v_A} [B]^{v_B} \sim P^{v_A} P^{v_B} \sim P^{v_A+v_B} \sim P^n \quad (\text{for example } A = \text{fuel}, B = \text{oxidant})$$

$$\dot{\omega} \sim \frac{1}{[A]_{\infty}} \frac{d[A]}{dt} \sim P^{-1} P^n \sim P^{n-1}$$

$$\text{Thus } S_L \sim \{\alpha \dot{\omega}\}^{1/2} \sim \{P^{-1} P^{n-1}\}^{1/2} \sim P^{(n-2)/2}$$

- For typical $n = 2$, S_L **independent of pressure**
- For “real” hydrocarbons, working backwards from experimental results, typically (e.g. stoichiometric CH_4 -air) $S_L \sim P^{-0.4}$, thus $n \approx 1.2$
- This suggests more reactions are one-body than two-body, but as discussed in the previous lecture, actually the observed n is due to competition between two-body $\text{H} + \text{O}_2$ branching vs. 3-body $\text{H} + \text{O}_2 + \text{M}$ which decelerates reaction

Deflagrations - temperature effect

- Since **Zeldovich number** (β) $\gg 1$

$$\beta \equiv \frac{T_{ad}}{\dot{\omega}(T_{ad})} \frac{\partial \dot{\omega}}{\partial T} \Big|_{T=T_{ad}} = \frac{E}{\Re T_{ad}}$$

For typical hydrocarbon-air flames, $E \approx 40$ kcal/mole

$\Re = 1.987$ cal/mole, $T_f \approx 2200\text{K}$ if adiabatic

$\Rightarrow \beta \approx 10$, at T close to T_f , $\omega \sim T^{10}$!!!

\Rightarrow Thin reaction zone concentrated near highest temp.

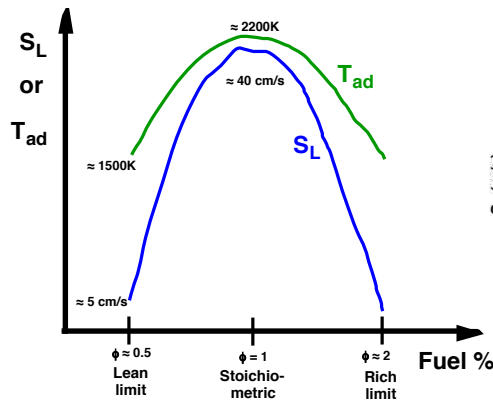
\therefore In Zeldovich (or any) estimate of S_L , overall reaction rate ω must be evaluated at T_{ad} , not T_{∞}

- \Rightarrow How can we estimate E ? If reaction rate depends more on E

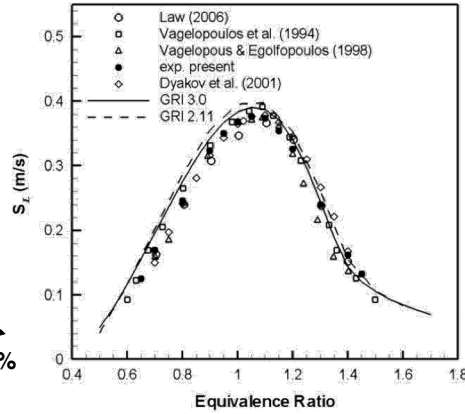
than concentrations $[]$, $S_L \sim (\alpha \dot{\omega})^{1/2} \sim \{\exp(-E/\Re T)\}^{1/2} \sim \exp(-E/2\Re T)$ - Plot of $\ln(S_L)$ vs. $1/T_{ad}$ has slope of $-E/2\Re$

- If β isn't large, then $\omega(T_{\infty}) \approx \omega(T_{ad})$ and reaction occurs even in the cold gases, so no control over flame is possible!
- Since $S_L \sim \omega^{1/2}$, $S_L \sim (T\beta)^{1/2} \sim T^5$ typically (that doesn't mean in every single case, just typically!)

Deflagrations – burning velocities



Schematic of flame temperatures and laminar burning velocities



Real data on S_L (CH_4 -air, 1 atm)

Deflagrations - summary

- These relations show the effect of T_{ad} (depends on fuel & stoichiometry), α (depends on diluent gas (usually N_2) & P), ω (depends on fuel, T , P) and pressure (engine condition) on laminar burning rates
- Re-emphasize: these estimates are based on an *overall reaction rate*; real flames have 1000s of individual reactions between 100s of species - but we can work backwards from experiments or detailed calculations to get these estimates for the overall reaction rate parameters

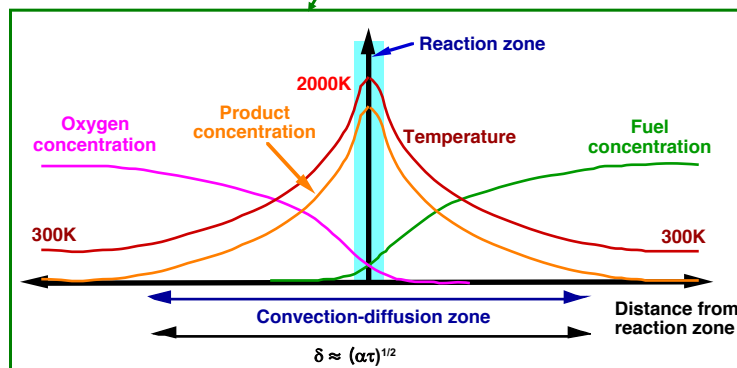
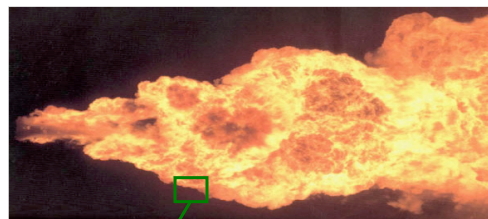
“Non-premixed” or “diffusion” flames

- Inherently safer – no mixing of fuel and oxidant except at time and place combustion is desired
- Slower than premixed – need to mix AND burn, not just burn
- Simplest approach to determining properties: “mixed is burned” - chemical reaction rates faster than mixing rates
- No inherent propagation rate (unlike premixed flames where $S_L \sim (\alpha\omega)^{1/2}$)
- No inherent thickness δ (unlike premixed flames where thickness $\sim \alpha/S_L$); in nonpremixed flames, determined by equating diffusion time scale δ^2/α to a characteristic flow time scale $\tau \Rightarrow \delta \sim (\alpha\tau)^{1/2}$ where $\tau = d/u$ for a jet, where d = diameter, u = velocity, L/u' for turbulent flow, $1/\Sigma$ for a counterflow etc.)
- Burning must occur near stoichiometric contour where reactant fluxes are in stoichiometric proportions (otherwise surplus of one reactant)
- Burning still must occur near highest T since $\omega \sim \exp(-E/RT)$ is very sensitive to temperature (like premixed flames)

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Nonpremixed flame structure

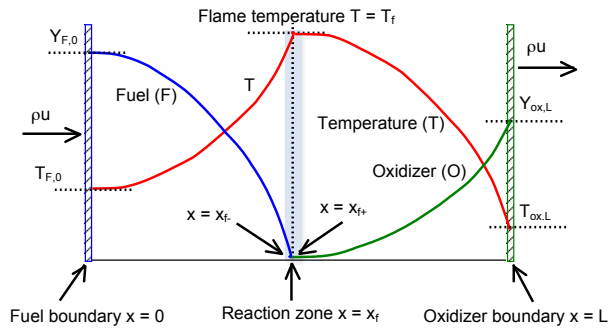


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1D planar steady nonpremixed flame

- Simplest non-premixed flame structure, highly contrived
- 1D flame, convection from left to right, unknowns T_f , x_f
- $\rho u = \text{const.}$ (mass conservation); assume ρD & $k/C_p = \text{const.}$



Fuel side: $u \frac{dT}{dx} - \frac{k}{\rho C_p} \frac{d^2 T}{dx^2} = 0$; $u \frac{dY_F}{dx} - D_F \frac{d^2 Y_F}{dx^2} = 0$

Oxidizer side: $u \frac{dT}{dx} - \frac{k}{\rho C_p} \frac{d^2 T}{dx^2} = 0$; $u \frac{dY_{ox}}{dx} - D_{ox} \frac{d^2 Y_{ox}}{dx^2} = 0$

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1D planar steady nonpremixed flame

- Fuel, oxidizer mass fractions

$$u \frac{dY_F}{dx} - D_F \frac{d^2 Y_F}{dx^2} = 0; \text{ boundary conditions } Y_F = Y_{F,0} \text{ at } x = 0, Y_F = 0 \text{ at } x = x_f$$

$$u \frac{dY_{ox}}{dx} - D_{ox} \frac{d^2 Y_{ox}}{dx^2} = 0; \text{ boundary conditions } Y_{ox} = Y_{ox,L} \text{ at } x = L, Y_{ox} = 0 \text{ at } x = x_f$$

$$\Rightarrow Y_F = Y_{F,0} \frac{1 - e^{(u/D_F)(x-x_f)}}{1 - e^{-(u/D_F)x_f}}; Y_{ox} = Y_{ox,L} \frac{1 - e^{(u/D_{ox})(x-x_f)}}{1 - e^{(u/D_{ox})(L-x_f)}}$$

Define non-dimensional parameters: $Pe = \frac{uL}{\alpha}$, $Le_{ox} = \frac{\alpha}{D_{ox}}$, $Le_F = \frac{\alpha}{D_F}$, $\tilde{x} = \frac{x}{L}$, $S = \frac{v_{ox} M_{ox} Y_{F,0}}{v_F M_F Y_{ox,L}}$

$$\Rightarrow \frac{Y_F}{Y_{F,0}} = \frac{1 - e^{-Pe Le_F (\tilde{x} - \tilde{x}_f)}}{1 - e^{-Pe Le_F \tilde{x}_f}}; \frac{Y_{ox}}{Y_{ox,L}} = \frac{1 - e^{Pe Le_{ox} (\tilde{x} - \tilde{x}_f)}}{1 - e^{Pe Le_{ox} (1 - \tilde{x}_f)}}$$

- Note that for $Pe \rightarrow 0$, $e^{Pe} \approx 1 + Pe$, thus Y profiles become linear

$$\frac{Y_F}{Y_{F,0}} = \frac{1 - e^{-Pe Le_F (\tilde{x} - \tilde{x}_f)}}{1 - e^{-Pe Le_F \tilde{x}_f}} \approx \frac{1 - (1 - Pe Le_F (\tilde{x} - \tilde{x}_f))}{1 - (1 - Pe Le_F \tilde{x}_f)} \approx 1 - \frac{\tilde{x}}{\tilde{x}_f}; \frac{Y_{ox}}{Y_{ox,L}} = \frac{1 - e^{Pe Le_{ox} (\tilde{x} - \tilde{x}_f)}}{1 - e^{Pe Le_{ox} (1 - \tilde{x}_f)}} \approx \frac{\tilde{x} - \tilde{x}_f}{1 - \tilde{x}_f}$$

- ... but how to determine flame location x_f ?

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1D planar steady nonpremixed flame

- For reaction $v_F \text{Fuel} + v_{Ox} \text{Ox} \rightarrow \text{products}$, flame location is where ratio of fuel to oxidizer mass fluxes due to diffusion is stoichiometric ratio = $v_F M_F / v_{Ox} M_{Ox}$ (but opposite directions, hence - sign) at $x = x_f$:

$$\begin{aligned} \rho D_F \frac{dY_F}{dx} \Big|_{x=x_{f-}} &= - \frac{v_F M_F}{v_{Ox} M_{Ox}} \rho D_{Ox} \frac{dY_{Ox}}{dx} \Big|_{x=x_{f+}} \\ \Rightarrow \frac{D_F Y_{F,0} e^{-(u/D_F)x_f}}{1 - e^{-(u/D_F)x_f}} \frac{u}{D_F} e^{(u/D_F)x_f} &= - \frac{v_F M_F}{v_{Ox} M_{Ox}} \frac{D_{Ox} Y_{Ox,L} e^{-(u/D_{Ox})x_f}}{1 - e^{(u/D_{Ox})(L-x_f)}} \frac{u}{D_{Ox}} \\ \Rightarrow \frac{1}{1 - e^{-(u/D_F)x_f}} &= - \frac{v_F M_F Y_{Ox,L}}{v_{Ox} M_{Ox} Y_{F,0}} \frac{1}{1 - e^{(u/D_{Ox})(L-x_f)}}; \text{ recall } S \equiv \frac{v_{Ox} M_{Ox} Y_{F,0}}{v_F M_F Y_{Ox,L}} \\ \Rightarrow S \left(1 - e^{(u/D_{Ox})(L-x_f)} \right) &= - \left(1 - e^{-(u/D_F)x_f} \right) \\ \Rightarrow S \left(1 - e^{(uL/\alpha)(\alpha/D_{Ox})(1-x_f/L)} \right) &= - \left(1 - e^{-(uL/\alpha)(\alpha/D_F)(x_f/L)} \right) \Rightarrow S \left(1 - e^{Pe_{Le_{Ox}}(1-\bar{x}_f)} \right) = - \left(1 - e^{-Pe_{Le_F}\bar{x}_f} \right) \\ \Rightarrow S e^{Pe_{Le_{Ox}}(1-\bar{x}_f)} + e^{-Pe_{Le_F}\bar{x}_f} &= S + 1 \text{ or } S = - \frac{1 - e^{-Pe_{Le_F}\bar{x}_f}}{1 - e^{Pe_{Le_{Ox}}(1-\bar{x}_f)}} \end{aligned}$$

1D planar steady nonpremixed flame

- Expression for flame position (x_f) not solvable in closed form but we can look at special cases (next page)
- x_f depends on the stoichiometric parameter (S), Lewis numbers of fuel and oxidant, and the strength of convection relative to diffusion as quantified by the Peclet number:

$$\frac{\text{Diffusion time scale}}{\text{Convection time scale}} \sim \frac{L^2 / \alpha}{L / u} = \frac{uL}{\alpha} \equiv Pe$$

- S is the ratio of mass of oxidizer stream to mass of fuel stream needed to make a stoichiometric mixture of the two
- Also often reported in non-premixed flame studies is the **stoichiometric mixture fraction** $Z_{st} = 1/(1+S)$ = mass fraction of fuel stream in a stoichiometric mixture of fuel and oxidant streams

1D planar steady nonpremixed flame

- Special case #1: weak convection ($Pe \rightarrow 0$, $\exp(Pe) \approx 1 + Pe$, throw out terms of order Pe^2)

$$Se^{PeLe_{ox}(1-\tilde{x}_f)} + e^{-PeLe_f\tilde{x}_f} = S+1 \Rightarrow S(1+PeLe_{ox}(1-\tilde{x}_f)) + 1 - PeLe_f\tilde{x}_f \approx S+1$$

$$SPeLe_{ox}(1-\tilde{x}_f) \approx PeLe_f\tilde{x}_f \Rightarrow \tilde{x}_f \approx \left(1 + \frac{Le_f}{SLe_{ox}}\right)^{-1} \Rightarrow x_f = L \left(1 + \frac{\nu_F M_F Y_{ox,L} Le_f}{\nu_{ox} M_{ox} Y_{F,0} Le_{ox}}\right)^{-1}$$

- Special case 2: $Le_f = Le_{ox} = 1$

$$Se^{Pe(1-\tilde{x}_f)} + e^{-Pe\tilde{x}_f} = S+1 \Rightarrow (Se^{Pe} + 1)e^{-Pe\tilde{x}_f} = S+1$$

$$\Rightarrow e^{-Pe\tilde{x}_f} = \frac{1+S}{1+Se^{Pe}} \Rightarrow \tilde{x}_f = \frac{1}{Pe} \ln\left(\frac{1+Se^{Pe}}{1+S}\right)$$

- Special case 3: $Pe \rightarrow \infty$

$$Se^{PeLe_{ox}(1-\tilde{x}_f)} + e^{-PeLe_f\tilde{x}_f} = S+1 \Rightarrow \tilde{x}_f \approx 1 - \frac{1}{PeLe_{ox}} \ln\left(\frac{1+S}{S}\right)$$

1D planar steady nonpremixed flame

- Energy equation:

$$\text{Fuel side: } u \frac{dT}{dx} - \frac{k}{\rho C_p} \frac{d^2T}{dx^2} = 0; \text{ BCs: } T = T_{F,0} \text{ at } x = 0, T = T_f \text{ at } x = x_f$$

$$\text{Oxidizer side: } u \frac{dT}{dx} - \frac{k}{\rho C_p} \frac{d^2T}{dx^2} = 0; \text{ BCs: } T = T_{ox,L} \text{ at } x = L, T = T_f \text{ at } x = x_f$$

- Solutions

$$\text{Fuel side: } T(x) = T_{F,0} + (T_f - T_{F,0}) \frac{1 - e^{(u/\alpha)x}}{1 - e^{(u/\alpha)x_f}} = T_{F,0} + (T_f - T_{F,0}) \frac{1 - e^{Pe\tilde{x}}}{1 - e^{Pe\tilde{x}_f}}$$

$$\text{Oxidizer side: } T = T_f - (T_f - T_{ox,L}) \frac{1 - e^{(u/\alpha)(x-x_f)}}{1 - e^{(u/\alpha)(L-x_f)}} = T_f - (T_f - T_{ox,L}) \frac{1 - e^{Pe(\tilde{x}-\tilde{x}_f)}}{1 - e^{Pe(1-\tilde{x}_f)}}$$

- Note again that as $Pe \rightarrow 0$, T profiles become linear

$$\text{Fuel side: } T(\tilde{x}) = T_{F,0} + (T_f - T_{F,0}) \frac{1 - e^{Pe\tilde{x}}}{1 - e^{Pe\tilde{x}_f}} \approx T_{F,0} + (T_f - T_{F,0}) \frac{\tilde{x}}{\tilde{x}_f}$$

$$\text{Oxidizer side: } T(\tilde{x}) = T_f - (T_f - T_{ox,L}) \frac{1 - e^{Pe(\tilde{x}-\tilde{x}_f)}}{1 - e^{Pe(1-\tilde{x}_f)}} \approx T_f - (T_f - T_{ox,L}) \frac{\tilde{x} - \tilde{x}_f}{1 - \tilde{x}_f}$$

1D planar steady nonpremixed flame

- Matching: heat release = (fuel flux to reaction zone) x (fuel heating value) = conductive heat flux away from reaction zone **on both sides**

$$\begin{aligned}
 -Q_R \rho D_F \left. \frac{dY_F}{dx} \right|_{x=x_{f-}} &= k \left. \frac{dT}{dx} \right|_{x=x_{f-}} - k \left. \frac{dT}{dx} \right|_{x=x_{f+}} \Rightarrow \\
 \frac{Q_R \rho D_F Y_{F,0} e^{-(u/D_F)x_f}}{1 - e^{-(u/D_F)x_f}} \frac{u}{D_F} e^{(ux/D_F)} &= -\frac{k(T_f - T_{F,0})}{1 - e^{(u/\alpha)x_f}} \frac{u}{\alpha} e^{(u/\alpha)x_f} - \frac{k(T_f - T_{ox,L})}{1 - e^{(u/\alpha)(L-x_f)}} \frac{u}{\alpha} e^{-(u/\alpha)x_f} \\
 \Rightarrow \frac{\rho Q_R Y_{F,0}}{1 - e^{-(u/D_F)x_f}} &= \frac{\rho C_p (T_f - T_{F,0})}{1 - e^{-(u/\alpha)x_f}} - \frac{\rho C_p (T_f - T_{ox,L})}{1 - e^{(u/\alpha)(L-x_f)}} \\
 \Rightarrow \frac{Q_R Y_{F,0}/C_p}{1 - e^{-(uL/\alpha)(x_f/L)}} &= \frac{T_f - T_{F,0}}{1 - e^{-(uL/\alpha)(x_f/L)}} - \frac{T_f - T_{ox,L}}{1 - e^{(uL/\alpha)(x_f/L)}} \\
 \Rightarrow \frac{Q_R Y_{F,0}/C_p}{1 - e^{-Pe Le_f \bar{x}_f}} &= \frac{T_f - T_{F,0}}{1 - e^{-Pe \bar{x}_f}} - \frac{T_f - T_{ox,L}}{1 - e^{Pe} e^{-Pe \bar{x}_f}}
 \end{aligned}$$

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- Can solve explicitly for T_f if you're desperate

$$\begin{aligned}
 \frac{Q_R Y_{F,0}/C_p}{1 - e^{-Pe Le_f \bar{x}_f}} &= \frac{T_f - T_{F,0}}{1 - e^{-Pe \bar{x}_f}} - \frac{T_f - T_{ox,L}}{1 - e^{Pe} e^{-Pe \bar{x}_f}} = \frac{T_f}{1 - e^{-Pe \bar{x}_f}} - \frac{T_{F,0}}{1 - e^{-Pe \bar{x}_f}} - \frac{T_f}{1 - e^{Pe} e^{-Pe \bar{x}_f}} + \frac{T_{ox,L}}{1 - e^{Pe} e^{-Pe \bar{x}_f}} \\
 T_f &= \frac{\frac{Q_R Y_{F,0}/C_p}{1 - e^{-Pe Le_f \bar{x}_f}} + \frac{T_{F,0}}{1 - e^{-Pe \bar{x}_f}} - \frac{T_{ox,L}}{1 - e^{Pe(1-\bar{x}_f)}}}{\frac{1}{1 - e^{-Pe \bar{x}_f}} - \frac{1}{1 - e^{Pe(1-\bar{x}_f)}}} \\
 \text{or } \tilde{T}_f &= \frac{\frac{1}{1 - e^{-Pe Le_f \bar{x}_f}} + \frac{\tilde{T}_{F,0}}{1 - e^{-Pe \bar{x}_f}} - \frac{\tilde{T}_{ox,L}}{1 - e^{Pe(1-\bar{x}_f)}}}{\frac{1}{1 - e^{-Pe \bar{x}_f}} - \frac{1}{1 - e^{Pe(1-\bar{x}_f)}}}; \tilde{T} \equiv \frac{C_p T}{Y_{F,0} Q_R}
 \end{aligned}$$

- ... looks wrong because T_f doesn't seem to depend on Le_{ox} , but recall x_f depends on Le_{ox} ! (Asymmetry in the above formula occurs because Q_R is the heating value per mass of FUEL not O_2)

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➤ Special case 1: $Pe \rightarrow 0$

$$\frac{Q_R Y_{F,0}/C_p}{1 - e^{-Pe \tilde{x}_f}} = \frac{T_f - T_{F,0}}{1 - e^{-Pe \tilde{x}_f}} - \frac{T_f - T_{ox,L}}{1 - e^{Pe} e^{-Pe \tilde{x}_f}} \Rightarrow \frac{Q_R Y_{F,0}/C_p}{1 - (1 - Pe Le_F \tilde{x}_f)} = \frac{T_f - T_{F,0}}{1 - (1 - Pe \tilde{x}_f)} - \frac{T_f - T_{ox,L}}{1 - (1 + Pe)(1 - Pe \tilde{x}_f)}$$

$$\Rightarrow \frac{Q_R Y_{F,0}/C_p}{Pe Le_F \tilde{x}_f} = \frac{T_f - T_{F,0}}{Pe \tilde{x}_f} - \frac{T_f - T_{ox,L}}{Pe(-1 + \tilde{x}_f)} \Rightarrow \frac{Q_R Y_{F,0}}{C_p Le_F} = (T_f - T_{F,0}) + (T_f - T_{ox,L}) \frac{\tilde{x}_f}{1 - \tilde{x}_f}$$

$$\text{Recall that as } Pe \rightarrow 0, \tilde{x}_f \approx \left(1 + \frac{Le_F}{S Le_{ox}}\right)^{-1} \Rightarrow \frac{Q_R Y_{F,0}}{C_p Le_F} = (T_f - T_{F,0}) + (T_f - T_{ox,L}) \frac{S Le_{ox}}{Le_F}$$

$$\Rightarrow \frac{Q_R}{C_p} = \frac{Le_F (T_f - T_{F,0})}{Y_{F,0}} + \frac{Le_{ox} (T_f - T_{ox,L})}{Y_{ox,0}} \frac{v_{ox} M_{ox}}{v_F M_F}$$

$$\text{or } T_f = \frac{Le_F}{S Le_{ox} + Le_F} \left(\frac{Q_R Y_{F,0}}{C_p Le_F} + T_{F,0} \right) + \frac{S Le_{ox}}{S Le_{ox} + Le_F} T_{ox,L}$$

- Dependence on Pe disappears (as expected)
- Behavior same on fuel and oxidant side except for stoichiometric scaling factor $v_{ox} M_{ox}/v_F M_F$ (also expected)
- **Decreasing Le has same effect as increasing reactant concentration (!)**
– completely unlike premixed flame where planar steady adiabatic flame temperature is independent of Le

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➤ Special case #2: $Le_F = Le_{ox} = 1$ (Pe not necessarily $\ll 1$)

$$\frac{Q_R Y_{F,0}/C_p}{1 - e^{-Pe \tilde{x}_f}} = \frac{T_f - T_{F,0}}{1 - e^{-Pe \tilde{x}_f}} - \frac{T_f - T_{ox,L}}{1 - e^{Pe} e^{-Pe \tilde{x}_f}}, e^{-Pe \tilde{x}_f} = \frac{1 + S}{1 + S e^{Pe}}$$

$$\Rightarrow \frac{Q_R Y_{F,0}}{C_p} = (T_f - T_{F,0}) - (T_f - T_{ox,L}) \frac{1 - e^{-Pe \tilde{x}_f}}{1 - e^{Pe} e^{-Pe \tilde{x}_f}} = (T_f - T_{F,0}) - (T_f - T_{ox,L}) \frac{1 - \frac{1 + S}{1 + S e^{Pe}}}{1 - e^{Pe} \frac{1 + S}{1 + S e^{Pe}}}$$

$$\Rightarrow \frac{Q_R Y_{F,0}}{C_p} = (T_f - T_{F,0}) - (T_f - T_{ox,L}) \frac{1 + S e^{Pe} - 1 - S}{1 + S e^{Pe} - e^{Pe} - S e^{Pe}} = (T_f - T_{F,0}) + (T_f - T_{ox,L}) S$$

$$\Rightarrow \frac{Q_R}{C_p} = \frac{T_f - T_{F,0}}{Y_{F,0}} + \frac{T_f - T_{ox,L}}{Y_{ox,L}} \frac{v_{ox} M_{ox}}{v_F M_F} \text{ or } T_f = \frac{\frac{Q_R Y_{F,0}}{C_p} + (T_{F,0} + S T_{ox,L})}{1 + S}$$

- When $Le_F = Le_{ox} = 1$, convection (contained in $Pe = uL/\alpha$) does not affect T_f at all!

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- Super special case 2a: $Le_F = Le_{ox} = 1$ AND $T_{F,0} = T_{ox,L} = T_\infty$:

$$\Rightarrow \frac{Q_R}{C_p} = \frac{T_f - T_\infty}{Y_{F,0}} + \frac{T_f - T_\infty}{Y_{ox,L}} \frac{\nu_{ox} M_{ox}}{\nu_F M_F} \Rightarrow T_f = \frac{Y_{F,0}}{1+S} \frac{Q_R}{C_p} + T_\infty$$

To interpret the $Y_{F,0}/(1+S)$ term, consider stoichiometric mixture of fuel and oxidizer streams:

$Y_{F,0}$ kg fuel, 1 kg total mixture from fuel side

$$\text{Need mass of oxidant} = Y_{F,0} \left(\frac{\text{mass of oxidant}}{\text{mass of fuel}} \right)_{\text{stoichiometric}} = Y_{F,0} \frac{\nu_{ox} M_{ox}}{\nu_F M_F} \text{ kg oxidizer}$$

$$\text{Total mass of oxidizer stream needed} = \frac{\text{mass of oxidant}}{Y_{ox,L}} = \frac{Y_{F,0} \frac{\nu_{ox} M_{ox}}{\nu_F M_F}}{Y_{ox,L}} \text{ kg of oxidizer stream}$$

$$\text{Mass fraction of fuel in this total mixture} = f = \frac{\text{mass of fuel}}{\text{total mass}} = \frac{Y_{F,0}}{Y_{F,0} \frac{\nu_{ox} M_{ox}}{\nu_F M_F} + 1 + \frac{Y_{F,0} \frac{\nu_{ox} M_{ox}}{\nu_F M_F}}{Y_{ox,L}}} = \frac{Y_{F,0}}{1 + \frac{Y_{F,0} \frac{\nu_{ox} M_{ox}}{\nu_F M_F}}{Y_{ox,L}}} = \frac{Y_{F,0}}{1+S}$$

$$\Rightarrow T_f = f \frac{Q_R}{C_p} + T_\infty - \text{adiabatic flame temperature of stoichiometric mixture of fuel stream + oxidant stream}$$

i.e. for $Le_F = Le_{ox} = 1$ and $T_{F,0} = T_{ox,L} = T_\infty$, the flame temperature is the same as a stoichiometric adiabatic PREMIXED flame, regardless of Pe

1D planar steady nonpremixed flame

- Special case 3: $Pe \rightarrow \infty$

$$\frac{Q_R Y_{F,0} / C_p}{1 - e^{-Pe Le_F \tilde{x}_f}} = \frac{T_f - T_{F,0}}{1 - e^{-Pe \tilde{x}_f}} - \frac{T_f - T_{ox,L}}{1 - e^{Pe} e^{-Pe \tilde{x}_f}} \Rightarrow \frac{Q_R Y_{F,0} / C_p}{1-0} = \frac{T_f - T_{F,0}}{1-0} - \frac{T_f - T_{ox,L}}{1 - e^{Pe(1-\tilde{x}_f)}}$$

$$\text{Recall as } Pe \rightarrow \infty: 1 - \tilde{x}_f \approx \frac{1}{Pe Le_{ox}} \ln \left(\frac{1+S}{S} \right) \Rightarrow Pe(1-\tilde{x}_f) = \ln \left(\frac{1+S}{S} \right)^{1/Le_{ox}}$$

$$\Rightarrow \frac{Q_R Y_{F,0}}{C_p} = (T_f - T_{F,0}) - \frac{T_f - T_{ox,L}}{1 - \left(\frac{1+S}{S} \right)^{1/Le_{ox}}} \Rightarrow T_f \text{ is independent of } Le_F$$

- As Pe (convection effects) increase, effects of Le_F & Le_{ox} on flame temperatures decrease – for $Pe \rightarrow \infty$ (flame pushed near oxidizer boundary), Le_F has no effect on T_f

1D planar steady nonpremixed flame

- Note that for nonpremixed flames, the ambient mass fractions of both fuel and O₂ (Y_{F,0} and Y_{ox,L} in this case) affect T_f because you're going to make a stoichiometric of the two, whereas for premixed flames only the mass fraction of the deficient reactant affects T_f significantly since the reactants are already mixed
- This is true of all nonpremixed flames, not just 1D planar steady ones

1D planar steady nonpremixed flame

- Much of our understanding of nonpremixed flames is contaminated by the facts that
 - Le_{ox} (O₂ in air) ≈ 1
 - We live in a concentrated fuel / diluted oxidizer world (S ≫ 1); recall that for Le_{ox} ≈ 1, at high Pe, T_f is unaffected by Pe or Le_F
 - Consider low Pe: for CH₄/air

$$S = \frac{v_{ox} M_{ox} Y_{F,0}}{v_F M_F Y_{ox,L}} = \frac{(2)(32)}{(1)(16)} \frac{1}{0.233} = 17.2 \gg 1$$

For $Pe \rightarrow 0, S \gg 1, Le_{ox} \approx 1$:

$$T_f = \frac{Le_F}{SLe_{ox} + Le_F} \left(\frac{Q_R Y_{F,0}}{C_p Le_F} + T_{F,0} \right) + \frac{SLe_{ox}}{SLe_{ox} + Le_F} T_{ox,L} \approx \frac{1}{S} \left(\frac{Q_R Y_{F,0}}{C_p} + T_{F,0} Le_F \right) + T_{ox,L}$$

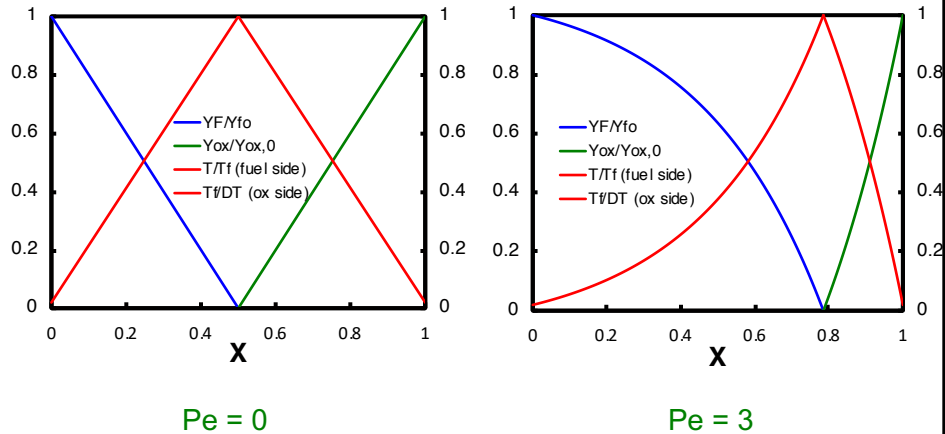
$$\frac{Q_R Y_{F,0}}{C_p} \approx \frac{(5 \times 10^7 \text{ J/kg})(1)}{1400 \text{ J/kgK}} \approx 35,700 \text{ K} \gg T_{F,0}$$

⇒ Le_F doesn't affect T_f significantly

- Thus we usually don't notice Le effects on T_f for nonpremixed flames (Le_F doesn't matter and Le_{O₂} ≈ 1)

Basic structure of nonpremixed flame

- The inevitable Excel spreadsheet ($S = 1$ and $Le_F = Le_{ox} = 1$ for the cases shown)



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- Alternative, "simpler" formulation for $Le_F = Le_{ox} = 1$ using **mixture fraction (Z)** (fraction of mixture that originated in fuel stream; $Z = 0$ at oxidizer boundary, $Z = 1$ at fuel boundary, $Z = Z_{st}$ at flame front)
- At any location x , mixture contains $Z(x)$ mass from fuel stream and $(1 - Z(x))$ mass from oxidizer stream:

$$Z = \frac{\text{Mass from fuel stream at } x}{\text{Total mass at } x} = \frac{\frac{Y_{ox,L} - Y_{ox}(x)}{v_{ox} M_{ox}} + \frac{Y_F(x)}{v_F M_F}}{\frac{Y_{ox,L} - Y_{ox}(x)}{v_{ox} M_{ox}} + \frac{Y_{ox}(x)}{v_F M_F} + \frac{Y_F(x)}{v_F M_F}} = \frac{\frac{Y_{ox,L} - Y_{ox}(x)}{Y_{ox,L}} + \frac{v_{ox} M_{ox} Y_{F,0}}{v_F M_F Y_{ox,L}} \frac{Y_F(x)}{Y_{F,0}}}{1 + \frac{v_{ox} M_{ox} Y_{F,0}}{v_F M_F Y_{ox,L}}}$$

$$= \frac{1 - \frac{Y_{ox}(x)}{Y_{ox,L}} + S \frac{Y_F(x)}{Y_{F,0}}}{1 + S}$$

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$$\frac{dZ}{dx} = \frac{1}{1+S} \left(S \frac{1}{Y_{F,0}} \frac{dY_F}{dx} - \frac{1}{Y_{Ox,L}} \frac{dY_{Ox}}{dx} \right); \frac{d^2Z}{dx^2} = \frac{1}{1+S} \left(S \frac{1}{Y_{F,0}} \frac{d^2Y_F}{dx^2} - \frac{1}{Y_{Ox,L}} \frac{d^2Y_{Ox}}{dx^2} \right)$$

$$u \frac{dY_F}{dx} - D_F \frac{d^2Y_F}{dx^2} = 0; u \frac{dY_{Ox}}{dx} - D_{Ox} \frac{d^2Y_{Ox}}{dx^2} = 0; Le_F = Le_{Ox} \Rightarrow D_F = D_{Ox} = D$$

$$\Rightarrow u \frac{S}{1+S} \frac{1}{Y_{F,0}} \frac{dY_F}{dx} - D \frac{S}{1+S} \frac{1}{Y_{F,0}} \frac{d^2Y_F}{dx^2} = 0; -u \frac{1}{1+S} \frac{1}{Y_{Ox,L}} \frac{dY_{Ox}}{dx} + D \frac{1}{1+S} \frac{1}{Y_{Ox,L}} \frac{d^2Y_{Ox}}{dx^2} = 0$$

$$\text{Add: } u \frac{d}{dx} \left(\frac{S}{1+S} \frac{1}{Y_{F,0}} \frac{dY_F}{dx} - \frac{1}{1+S} \frac{1}{Y_{Ox,L}} \frac{dY_{Ox}}{dx} \right) - D \frac{d^2}{dx^2} \left(\frac{S}{1+S} \frac{1}{Y_{F,0}} \frac{dY_F}{dx} - \frac{1}{1+S} \frac{1}{Y_{Ox,L}} \frac{dY_{Ox}}{dx} \right) = 0$$

$$\Rightarrow u \frac{dZ}{dx} - D \frac{d^2Z}{dx^2} = 0;$$

Boundary conditions $Z = 1$ at $x = 0$, $Z = 0$ at $x = L \Rightarrow Z(\tilde{x}) = \frac{e^{Pe\tilde{x}} - e^{Pe}}{1 - e^{Pe}}; \tilde{x} \equiv \frac{x}{L}, Pe \equiv \frac{uL}{D}$

At flame front $Z(\tilde{x}_f) = Z_{st} = \frac{1}{1+S} \Rightarrow \tilde{x}_f = \frac{1}{Pe} \ln \left(\frac{1 + Se^{Pe}}{1+S} \right)$ as before

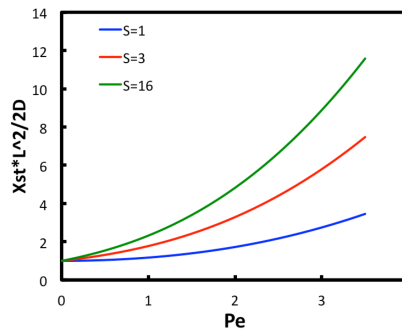
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- Z formulation does not require fuel and oxidant to react at $x = x_f$ or anyplace for that matter, so is especially useful for near-extinction conditions where fuel or oxidant leakage may occur
- Strength of reactant fluxes to reaction zone characterized by **scalar dissipation** (χ , units 1/time), most useful to evaluate at flame location (χ_f) where reaction occurs:

$$\chi \equiv 2D \left(\frac{dZ}{dx} \right)^2 = \frac{2D}{L^2} \left(\frac{dZ}{d\tilde{x}} \right)^2 = \frac{2D}{L^2} \left(\frac{Pe (e^{Pe\tilde{x}})}{1 - e^{Pe}} \right)^2;$$

$$\chi_f = \frac{2D}{L^2} \left(\frac{Pe \left(\frac{1 + Se^{Pe}}{1+S} \right)}{1 - e^{Pe}} \right)^2 = \frac{2D}{L^2} \left(\frac{Pe(1 + Se^{Pe})}{(1+S)(1 - e^{Pe})} \right)^2$$

- Both increasing Pe and S increase χ_f and thus weaken flame (by symmetry, negative Pe and $S \ll 1$ would also be a weak condition)



1D planar steady nonpremixed flame

- Note also

$$Z(\tilde{x}) = \frac{e^{Pe \tilde{x}} - e^{Pe}}{1 - e^{Pe}} \Rightarrow e^{Pe \tilde{x}} = Z(\tilde{x})[1 - e^{Pe}] + e^{Pe}; \tilde{x}_f = \frac{1}{Pe} \ln\left(\frac{1 + Se^{Pe}}{1 + S}\right) \Rightarrow e^{Pe \tilde{x}_f} = \frac{1 + Se^{Pe}}{1 + S}$$

$$\text{Fuel side: } T(\tilde{x}) = T_{F,0} + (T_f - T_{F,0}) \frac{1 - e^{Pe \tilde{x}}}{1 - e^{Pe \tilde{x}_f}} = T_{F,0} + (T_f - T_{F,0}) \frac{1 - Z(\tilde{x})[1 - e^{Pe}] - e^{Pe}}{1 - \frac{1 + Se^{Pe}}{1 + S}}$$

$$\Rightarrow T(Z) = T_{F,0} + (T_f - T_{F,0}) (1 - Z) \frac{1 + S}{S}$$

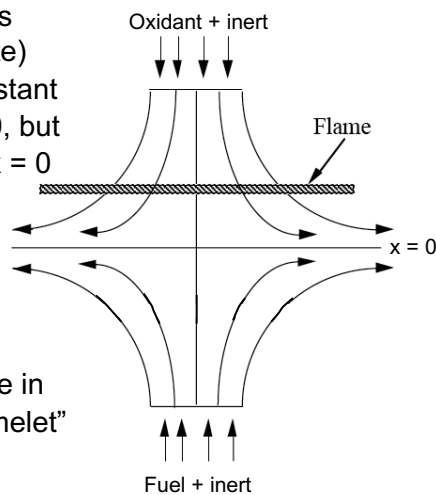
$$\text{Oxidizer side: } T(\tilde{x}) = T_f - (T_f - T_{ox,L}) \frac{1 - e^{Pe(\tilde{x} - \tilde{x}_f)}}{1 - e^{Pe(1 - \tilde{x}_f)}} = T_f - (T_f - T_{ox,L}) \frac{1 - e^{Pe \tilde{x}} e^{-Pe \tilde{x}_f}}{1 - e^{Pe} e^{-Pe \tilde{x}_f}}$$

$$= T_f - (T_f - T_{ox,L}) \frac{1 + Se^{Pe} - (Z(\tilde{x})[1 - e^{Pe}] + e^{Pe})(1 + S)}{1 - e^{Pe}} = T_f - (T_f - T_{ox,L}) [1 - Z(1 + S)]$$

- Temperature (and composition) profiles are linear when plotted vs. Z instead of vs. x – huge simplification
- Applies to other flows (stretched counterflow, droplet, ...) if $Le_F = Le_{ox} = 1$

1D stretched flame

- Simple counterflow, fuel at $x = -\infty$, oxidant at $x = +\infty$
- Velocity (u) is not constant in this case, now $u = -\Sigma x$ (Σ = strain rate)
- Again assume ρD & k/C_p = constant
- Stagnation plane ($u = 0$) at $x = 0$, but flame may be on either side of $x = 0$ depending on S , Le_F & Le_{ox}
- Somewhat similar to plane unstretched case but this configuration is easy to obtain experimentally
- Model for local behavior of flame in turbulent flow field ("laminar flamelet" model)



1D stretched flame

➤ Species conservation:

$$\rho u \frac{dY_F}{dx} - \rho D \frac{d^2Y_F}{dx^2} = 0 \Rightarrow -\Sigma x \frac{dY_F}{dx} - \alpha Le \frac{d^2Y_F}{dx^2} = 0;$$

$$\text{Let } \tilde{x} = \frac{x}{\sqrt{2\alpha/\Sigma}} \Rightarrow \tilde{x} \frac{dY_F}{d\tilde{x}} + \frac{1}{2Le_F} \frac{d^2Y_F}{d\tilde{x}^2} = 0 \Rightarrow Y_F(\tilde{x}) = C_1 \operatorname{erf}(\sqrt{Le_F} \tilde{x}) + C_2$$

$$\text{Recall } \operatorname{erf}(a) = \frac{2}{\sqrt{\pi}} \int_0^a e^{-t^2} dt$$

Fuel side boundary conditions: $\tilde{x} = \tilde{x}_f, Y_F = 0; \tilde{x} = -\infty, Y_F = Y_{F,-\infty}$

$$\Rightarrow Y_F(\tilde{x}) = \frac{Y_{F,-\infty} \left(\operatorname{erf}(\sqrt{Le_F} \tilde{x}_f) - \operatorname{erf}(\sqrt{Le_F} \tilde{x}) \right)}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)}; \left. \frac{dY_F}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f} = -\frac{2\sqrt{Le_F}}{\sqrt{\pi}} \frac{Y_{F,-\infty} e^{-Le_F \tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)}$$

Oxidizer side boundary conditions: $\tilde{x} = \tilde{x}_f, Y_{ox} = 0; \tilde{x} = \infty, Y_{ox} = Y_{ox,\infty}$

$$\Rightarrow Y_{ox}(\tilde{x}) = -\frac{Y_{ox,\infty} \left(\operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f) - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}) \right)}{1 - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f)}; \left. \frac{dY_{ox}}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f} = \frac{2\sqrt{Le_{ox}}}{\sqrt{\pi}} \frac{Y_{ox,\infty} e^{-Le_{ox} \tilde{x}_f^2}}{1 - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f)}$$

1D stretched flame

➤ Energy equation:

$$\rho u C_p \frac{dT}{dx} - k \frac{d^2T}{dx^2} = 0 \Rightarrow -\Sigma x \frac{dT}{dx} - \alpha \frac{d^2T}{dx^2} = 0;$$

$$\text{Again let } \tilde{x} = \frac{x}{\sqrt{2\alpha/\Sigma}} \Rightarrow \tilde{x} \frac{dT}{d\tilde{x}} + \frac{1}{2} \frac{d^2T}{d\tilde{x}^2} = 0 \Rightarrow T(\tilde{x}) = C_1 \operatorname{erf}(\tilde{x}) + C_2$$

Fuel side boundary conditions: $\tilde{x} = \tilde{x}_f, T = T_f; \tilde{x} = -\infty, T = T_{F,-\infty}$

$$\Rightarrow T(\tilde{x}) = \frac{(T_f - T_{F,-\infty}) \operatorname{erf}(\tilde{x}) + T_{F,-\infty} \operatorname{erf}(\tilde{x}_f) + T_f}{1 + \operatorname{erf}(\tilde{x}_f)}; \left. \frac{dT}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f} = \frac{2(T_f - T_{F,-\infty}) e^{-\tilde{x}_f^2}}{\sqrt{\pi} (1 + \operatorname{erf}(\tilde{x}_f))}$$

Oxidizer side boundary conditions: $\tilde{x} = \tilde{x}_f, T = T_f; \tilde{x} = +\infty, T = T_{ox,\infty}$

$$\Rightarrow T(\tilde{x}) = -\frac{(T_f - T_{ox,\infty}) \operatorname{erf}(\tilde{x}) + T_{ox,\infty} \operatorname{erf}(\tilde{x}_f) - T_f}{1 - \operatorname{erf}(\tilde{x}_f)}; \left. \frac{dT}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f} = -\frac{2(T_f - T_{ox,\infty}) e^{-\tilde{x}_f^2}}{\sqrt{\pi} (1 - \operatorname{erf}(\tilde{x}_f))}$$

1D stretched flame

➤ Stoichiometric balance at flame sheet is same as always

$$\begin{aligned} \rho D_F \left. \frac{dY_F}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f^-} &= -\frac{v_F M_F}{v_{ox} M_{ox}} \rho D_{ox} \left. \frac{dY_{ox}}{d\tilde{x}} \right|_{\tilde{x}=\tilde{x}_f^+} \\ -\rho D_F \frac{2\sqrt{Le_F}}{\sqrt{\pi}} \frac{Y_{F,-\infty} e^{-Le_F \tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)} &= +\frac{v_F M_F}{v_{ox} M_{ox}} \rho D_{ox} \frac{2\sqrt{Le_{ox}}}{\sqrt{\pi}} \frac{Y_{ox,\infty} e^{-Le_{ox} \tilde{x}_f^2}}{1 - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f)} \\ \Rightarrow \frac{D_F}{D_{ox}} \sqrt{\frac{Le_F}{Le_{ox}}} \frac{e^{-Le_F \tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)} &= \frac{v_F M_F Y_{ox,\infty}}{v_{ox} M_{ox} Y_{F,-\infty}} \frac{e^{-Le_{ox} \tilde{x}_f^2}}{1 - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f)} \\ \Rightarrow S \sqrt{\frac{Le_{ox}}{Le_F}} e^{-(Le_F - Le_{ox}) \tilde{x}_f^2} &= \frac{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)}{1 - \operatorname{erf}(\sqrt{Le_{ox}} \tilde{x}_f)} \end{aligned}$$

In general, not solvable for \tilde{x}_f in closed form but if $Le_F = Le_{ox} = 1$ then

$$S = \frac{1 + \operatorname{erf}(\tilde{x}_f)}{1 - \operatorname{erf}(\tilde{x}_f)} \Rightarrow \tilde{x}_f = \operatorname{erf}^{-1}\left(\frac{S-1}{S+1}\right)$$

➤ Note that no flow parameter (like Pe) appears explicitly; strain rate Σ absorbed into scaling of \tilde{x}_f

1D stretched flame

➤ Energy balance condition is the same as always

$$\begin{aligned} -Q_R \rho D_F \left. \frac{dY_F}{dx} \right|_{x=x_f^-} &= k \left. \frac{dT}{dx} \right|_{x=x_f^-} - k \left. \frac{dT}{dx} \right|_{x=x_f^+} \\ \Rightarrow +Q_R \rho D_F \frac{2\sqrt{Le_F}}{\sqrt{\pi}} \frac{Y_{F,-\infty} e^{-Le_F \tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)} &= k \frac{2}{\sqrt{\pi}} \frac{(T_f - T_{F,-\infty}) e^{-\tilde{x}_f^2}}{1 + \operatorname{erf}(\tilde{x}_f)} + k \frac{2}{\sqrt{\pi}} \frac{(T_f - T_{ox,+\infty}) e^{-\tilde{x}_f^2}}{1 - \operatorname{erf}(\tilde{x}_f)} \\ \Rightarrow \frac{Y_{F,-\infty} Q_R}{C_p} \frac{\rho C_p D_F}{k} \sqrt{Le_F} \frac{e^{-Le_F \tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)} &= \frac{(T_f - T_{F,-\infty}) e^{-\tilde{x}_f^2}}{1 + \operatorname{erf}(\tilde{x}_f)} + \frac{(T_f - T_{ox,+\infty}) e^{-\tilde{x}_f^2}}{1 - \operatorname{erf}(\tilde{x}_f)} \\ \Rightarrow \frac{Y_{F,-\infty} Q_R}{C_p} \frac{1}{\sqrt{Le_F}} \frac{e^{(1-Le_F)\tilde{x}_f^2}}{1 + \operatorname{erf}(\sqrt{Le_F} \tilde{x}_f)} &= \frac{T_f - T_{F,-\infty}}{1 + \operatorname{erf}(\tilde{x}_f)} + \frac{T_f - T_{ox,+\infty}}{1 - \operatorname{erf}(\tilde{x}_f)} \end{aligned}$$

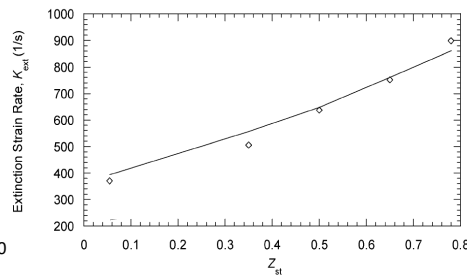
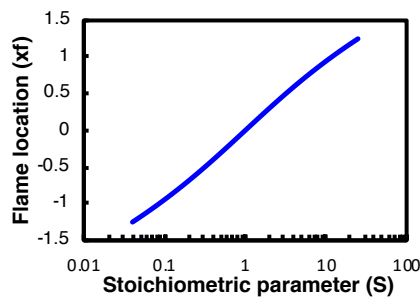
1D stretched flame

➤ Energy balance continued...

$$\begin{aligned} \text{If } Le_F = Le_{ox} = 1 \text{ then } \frac{Y_{F,-\infty} Q_R}{C_P} &= (T_f - T_{F,-\infty}) + (T_f - T_{ox,+\infty}) \frac{1 + \operatorname{erf}(\tilde{x}_f)}{1 - \operatorname{erf}(\tilde{x}_f)} \\ &= (T_f - T_{F,-\infty}) + (T_f - T_{ox,+\infty}) \frac{1 + \frac{S-1}{S+1}}{1 - \frac{S-1}{S+1}} \\ \Rightarrow \frac{Y_{F,-\infty} Q_R}{C_P} &= (T_f - T_{F,-\infty}) + (T_f - T_{ox,+\infty}) S \text{ or } T_f = \frac{\frac{Q_R Y_{F,-\infty}}{C_P} + (T_{F,-\infty} + S T_{ox,+\infty})}{1 + S} \end{aligned}$$

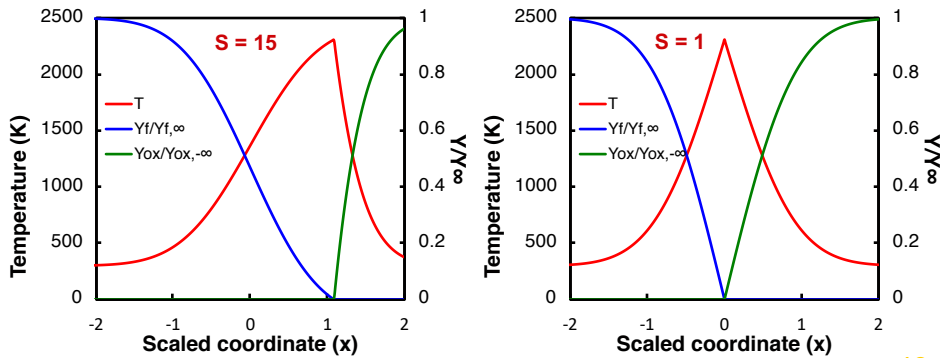
1D stretched flame

- For $S = 1$, $Le_F = Le_{ox} = 1$, flame located at stagnation plane
- For $S > 1$ (oxidizer more diluted than fuel), flame moves toward oxidizer boundary – need steeper gradient of oxidizer
- (Chemical effect, not predictable with 1-step chemistry): S or $Z_{st} = 1/(1+S)$ has significant effect; for flame on oxidizer side (large S , small Z_{st}) radicals (mostly formed on fuel side because of lower C-H & C-C bond strengths compared to O=O) are convected away from flame sheet, so flames are weaker even for same T_f (Chen & Axelbaum 2005)



1D stretched flame

- Temperature & species profiles are error functions
- For $S = 1$, profiles are symmetric about $x = 0$; convection effect (u) is small at flame location & behavior similar to unstretched flame at low Pe , decreasing either Le increases T_f
- For $S > 1$, flame lies on oxidizer side of stagnation plane; flame temperature affected mostly by Le_{ox} but not Le_F ; decreasing Le_F moves flame closer to $x = 0$ & increases T_f



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1D stretched flame

- Mixture fraction formulation for $Le_F = Le_{O_2} = 1$

$$Z = \frac{1 - \frac{Y_{ox}(x)}{Y_{ox,L}} + S \frac{Y_F(x)}{Y_{F,0}}}{1+S}; Le_F = Le_{ox} = 1; \text{ let } \tilde{x} = \frac{x}{\sqrt{2D/\Sigma}} \Rightarrow \tilde{x} \frac{dZ}{d\tilde{x}} + \frac{1}{2} \frac{d^2Z}{d\tilde{x}^2} = 0$$

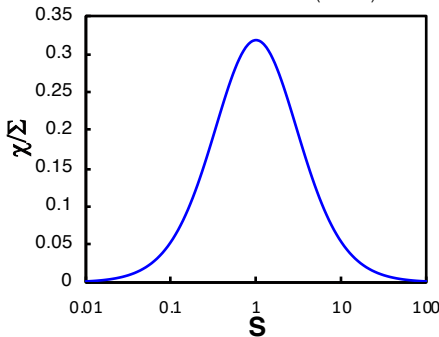
$$\Rightarrow Z(\tilde{x}) = C_1 \text{erf}(\tilde{x}) + C_2; \text{ boundary conditions } Z = 1 \text{ at } x = -\infty, Z = 0 \text{ at } x = +\infty$$

$$\Rightarrow Z(\tilde{x}) = \frac{1 - \text{erf}(\tilde{x})}{2}; \text{ at flame front } Z(\tilde{x}_f) = Z_{st} = \frac{1}{1+S} \Rightarrow \tilde{x}_f = \text{erf}^{-1}\left(\frac{S-1}{S+1}\right) \text{ as before}$$

$$\chi = 2D \left(\frac{dZ}{dx} \right)^2 = 2D \left(\frac{dZ}{d\tilde{x}} \frac{d\tilde{x}}{dx} \right)^2$$

$$= 2D \left(-\frac{1}{2} \frac{2e^{-\tilde{x}^2}}{\sqrt{\pi}} \frac{1}{\sqrt{2D/\Sigma}} \right)^2 = \frac{\Sigma}{\pi} e^{-2\tilde{x}^2}$$

$$\chi_f = \frac{\Sigma}{\pi} \exp \left[-2 \left(\text{erf}^{-1} \left(\frac{S-1}{S+1} \right) \right)^2 \right]$$

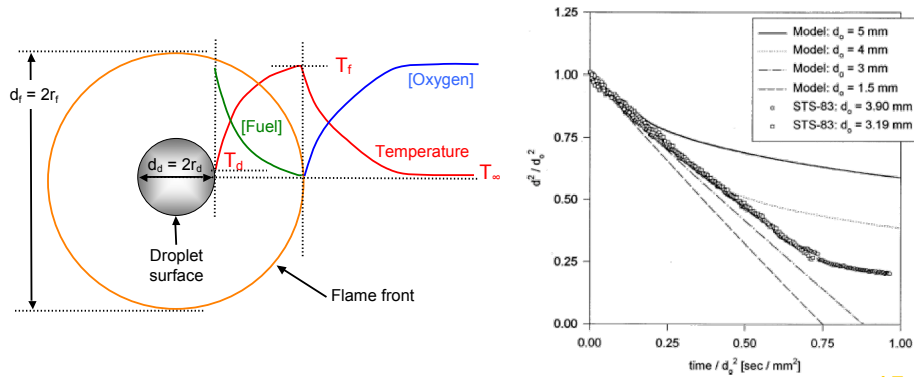


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Droplet combustion

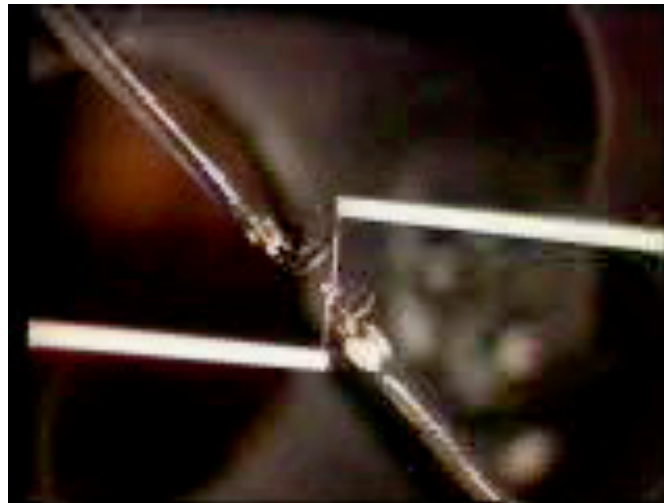
- Heat from flame conducted to fuel surface, vaporizes fuel, fuel convects/diffuses to flame front, O_2 diffuses to flame front from outside, burning occurs at stoich. location
- As fuel burns, droplet diameter $d_d(t)$ decreases until $d_d = 0$ or droplet may extinguish before reaching $d_d = 0$
- Experiments typically show $d_d(0)^2 - d_d(t)^2 \approx Kt$



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Droplet combustion



Marchese et al. (1999), space experiments, heptane in O_2 -He

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Droplet combustion

- Analysis similar to 1D planar flame cases already discussed but need to use 1D steady **spherical** version of convection-diffusion conservation equations for Y_f , Y_{ox} and T

$$\text{Mass conservation: } \frac{\partial \rho}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u}) = 0 \Rightarrow \frac{1}{r^2} \frac{d}{dr} (r^2 \rho u) = 0$$

$$\Rightarrow \dot{m} = 4\pi r^2 \rho u = \text{constant (compared to } \rho u = \text{constant for planar case)}$$

$$\text{Energy conservation: } \rho \left[\frac{\partial h}{\partial t} + (\bar{u} \cdot \bar{\nabla} h) \right] - \bar{\nabla} \cdot (k \bar{\nabla} T) = \dot{q}''' \Rightarrow \rho C_p \bar{u} \cdot \bar{\nabla} T - k \bar{\nabla} \cdot \bar{\nabla} T = 0$$

$$\Rightarrow \rho C_p u \frac{dT}{dr} - \frac{k}{r^2} \frac{d}{dr} \left(r^2 \frac{dT}{dr} \right) = 0$$

$$\text{Species conservation: } \rho \left[\frac{\partial Y_i}{\partial t} + (\bar{u} \cdot \bar{\nabla} Y_i) \right] - \bar{\nabla} \cdot (\rho D \bar{\nabla} Y_i) = M_i \dot{\omega}_i \Rightarrow \rho \bar{u} \cdot \bar{\nabla} Y_i - \bar{\nabla} \cdot (\rho D \bar{\nabla} Y_i) = 0$$

$$\Rightarrow \rho u \frac{dY_i}{dr} - \frac{\rho D}{r^2} \frac{d}{dr} \left(r^2 \frac{dY_i}{dr} \right) = 0$$

Droplet combustion

- Unknowns
 - Flame temperature T_f and flame location r_f (as with gaseous flame cases previously discussed)
 - Fuel mass flux $\dot{m} = \rho u A = \rho_d u_d (4\pi r_d^2)$ from droplet surface (expressed in Pe in the following analysis) (**new, was a known quantity in previous cases**)
 - » Note that \dot{m} must be constant, but the fuel mass flow is not; the fuel disappears by $r = r_f$, but the total mass flow (i.e. of inert and products) must be constant out to $r = \infty$
 - Fuel concentration at droplet surface $Y_{F,d}$ or stoichiometric parameter S (**new, was a known quantity in previous cases**)
 - 2 more unknowns, so need 2 more equations (total of 4)
 - » Reactant diffusive fluxes into flame sheet in stoichiometric proportions (same as gaseous flames)
 - » Fuel enthalpy flux into flame sheet = thermal enthalpy flux out (by heat conduction) (same as gaseous flames)
 - » Energy balance at droplet surface (**new**)
 - » Mass balance at droplet surface (**new**)

Droplet combustion

- Fuel side ($r_d \leq r \leq r_f$)

$$\rho u \frac{dY_F}{dr} - \frac{\rho D_F}{r^2} \frac{d}{dr} \left(r^2 \frac{dY_F}{dr} \right) = 0, \dot{m} = 4\pi r^2 \rho u = \text{constant}$$

$$\Rightarrow PeLe_F \frac{dY_F}{d\tilde{r}} = \frac{d}{d\tilde{r}} \left(\tilde{r}^2 \frac{dY_F}{d\tilde{r}} \right) \text{ where } Pe \equiv \frac{\dot{m} C_p}{4\pi k r_d}, \tilde{r} \equiv \frac{r}{r_d}$$

$$\Rightarrow PeLe_F Y_F + C_1 = \tilde{r}^2 \frac{dY_F}{d\tilde{r}} \Rightarrow \frac{dY_F}{PeLe_F Y_F + C_1} = \frac{d\tilde{r}}{\tilde{r}^2}$$

$$\Rightarrow \frac{\ln(PeLe_F Y_F + C_1)}{PeLe_F} = -\frac{1}{\tilde{r}} + C_2 \Rightarrow Y_F = C_1' + C_2' e^{-PeLe_F/\tilde{r}}$$

Boundary Conditions: $r = r_d$ ($\tilde{r} = 1$), $Y_F = Y_{F,d}$ and $r = r_f$ ($\tilde{r} = \tilde{r}_f$), $Y_F = 0$

$$\Rightarrow Y_F(\tilde{r}) = \frac{Y_{F,d} \left(e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F/\tilde{r}} \right)}{e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F}}; \frac{dY_F}{d\tilde{r}} = -\frac{PeLe_F}{\tilde{r}^2} \frac{Y_{F,d} e^{-PeLe_F/\tilde{r}}}{e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F}}$$

$$\left. \frac{dY_F}{d\tilde{r}} \right|_{\tilde{r}=1} = -PeLe_F \frac{Y_{F,d} e^{-PeLe_F}}{e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F}} = -PeLe_F \frac{Y_{F,d}}{e^{PeLe_F(1-1/\tilde{r}_f)} - 1}$$

$$\left. \frac{dY_F}{d\tilde{r}} \right|_{\tilde{r}=\tilde{r}_f} = \frac{PeLe_F}{\tilde{r}_f^2} \frac{Y_{F,d}}{e^{-PeLe_F(1-1/\tilde{r}_f)} - 1}$$

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Droplet combustion

- Note similarities to planar case, but now due to r^2 factors in conservation equations we have $\exp(-Pe/r)$ terms instead of $\exp(-Pe \cdot x)$ terms
- Oxygen side ($r \geq r_f$)

$$Y_{ox} = C_1' + C_2' e^{-PeLe_{ox}/\tilde{r}}$$

Boundary Conditions: $r = r_f$ ($\tilde{r} = \tilde{r}_f$), $Y_{ox} = 0$ and $\tilde{r} \rightarrow \infty$, $Y_{ox} = Y_{ox,\infty}$

$$\Rightarrow Y_{ox}(\tilde{r}) = Y_{ox,\infty} \frac{e^{-PeLe_{ox}/\tilde{r}} - e^{-PeLe_{ox}/\tilde{r}_f}}{1 - e^{-PeLe_{ox}/\tilde{r}_f}}; \frac{dY_{ox}}{d\tilde{r}} = Y_{ox,\infty} \frac{PeLe_{ox}}{\tilde{r}^2} \frac{e^{-PeLe_{ox}/\tilde{r}}}{1 - e^{-PeLe_{ox}/\tilde{r}_f}}$$

$$\left. \frac{dY_{ox}}{d\tilde{r}} \right|_{\tilde{r}=\tilde{r}_f} = \frac{PeLe_{ox}}{\tilde{r}_f^2} \frac{Y_{ox,\infty}}{e^{PeLe_{ox}/\tilde{r}_f} - 1}; \left. \frac{dY_{ox}}{d\tilde{r}} \right|_{\tilde{r}=\infty} = 0$$

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Droplet combustion

- Temperature ($r_d \leq r \leq r_f$)

$$\rho C_p u \frac{dT}{dr} - \frac{k}{r^2} \frac{d}{dr} \left(r^2 \frac{dT}{dr} \right) = 0, \dot{m} = 4\pi r^2 \rho u \Rightarrow Pe \frac{dT}{d\tilde{r}} = \frac{d}{d\tilde{r}} \left(\tilde{r}^2 \frac{dT}{d\tilde{r}} \right)$$

$$\Rightarrow PeT + C_1 = r^2 \frac{dT}{dr} \Rightarrow T = C_1' + C_2' e^{-Pe/r}, \text{ BCs: } \tilde{r} = 1, T = T_d \text{ and } \tilde{r} = \tilde{r}_f, T = T_f$$

$$\Rightarrow T(\tilde{r}) = \frac{(T_f - T_d) e^{-Pe/\tilde{r}} - (T_f e^{-Pe} - T_d e^{-Pe/\tilde{r}_f})}{e^{-Pe/\tilde{r}_f} - e^{-Pe}}, \frac{dT}{d\tilde{r}} = \frac{Pe (T_f - T_d) e^{-Pe/\tilde{r}}}{\tilde{r}^2 (e^{-Pe/\tilde{r}_f} - e^{-Pe})}$$

$$\left. \frac{dT}{dr} \right|_{\tilde{r}=1} = Pe \frac{(T_f - T_d) e^{-Pe}}{e^{-Pe/\tilde{r}_f} - e^{-Pe}} = Pe \frac{T_f - T_d}{e^{Pe(1-1/\tilde{r}_f)} - 1}, \left. \frac{dT}{dr} \right|_{\tilde{r}=\tilde{r}_f} = \frac{Pe (T_f - T_d)}{\tilde{r}_f^2 (1 - e^{-Pe(1-1/\tilde{r}_f)})}$$

- Temperature ($r \geq r_f$)

$$PeT + C_1 = \tilde{r}^2 \frac{dT}{d\tilde{r}} \Rightarrow T = C_1' + C_2' e^{-Pe/\tilde{r}}, \text{ BCs: } \tilde{r} \rightarrow \infty, T = T_\infty \text{ and } \tilde{r} = \tilde{r}_f, T = T_f$$

$$\Rightarrow T(\tilde{r}) = \frac{(T_f - T_\infty) e^{-Pe/\tilde{r}_f} - (T_f - T_\infty) e^{-Pe/\tilde{r}}}{1 - e^{-Pe/\tilde{r}_f}}, \frac{dT}{d\tilde{r}} = -\frac{Pe (T_f - T_\infty) e^{-Pe/\tilde{r}}}{\tilde{r}^2 (1 - e^{-Pe/\tilde{r}_f})}$$

$$\left. \frac{dT}{d\tilde{r}} \right|_{\tilde{r}=\tilde{r}_f} = -\frac{Pe (T_f - T_\infty) e^{-Pe/\tilde{r}_f}}{\tilde{r}_f^2 (1 - e^{-Pe/\tilde{r}_f})} = -\frac{Pe (T_f - T_\infty)}{\tilde{r}_f^2 (e^{Pe/\tilde{r}_f} - 1)}, \left. \frac{dT}{d\tilde{r}} \right|_{\tilde{r}=\infty} = 0$$

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Droplet combustion

- As with flat flame, stoichiometric balance at flame sheet is

$$\rho D_F \left. \frac{dY_F}{d\tilde{r}} \right|_{\tilde{r}=\tilde{r}_{f-}} = -\frac{\nu_F M_F}{\nu_{ox} M_{ox}} \rho D_{ox} \left. \frac{dY_{ox}}{d\tilde{r}} \right|_{\tilde{r}=\tilde{r}_{f+}}$$

$$\rho D_F \frac{Pe Le_F}{\tilde{r}_f^2} \frac{Y_{F,d}}{e^{-Pe Le_F (1-1/\tilde{r}_f)} - 1} = -\frac{\nu_F M_F}{\nu_{ox} M_{ox}} \rho D_{ox} \frac{Pe Le_{ox}}{\tilde{r}_f^2} \frac{Y_{ox,\infty}}{e^{Pe Le_{ox}/\tilde{r}_f} - 1}$$

$$\frac{1}{e^{-Pe Le_F (1-1/\tilde{r}_f)} - 1} = -\frac{\nu_F M_F Y_{ox,\infty}}{\nu_{ox} M_{ox} Y_{F,d}} \frac{1}{e^{Pe Le_{ox}/\tilde{r}_f} - 1} = -\frac{1}{S} \frac{1}{e^{Pe Le_{ox}/\tilde{r}_f} - 1}$$

$$\Rightarrow e^{Pe Le_F (1/\tilde{r}_f - 1)} + S e^{Pe Le_{ox}/\tilde{r}_f} = 1 + S \quad (\text{Eq. 1})$$

- Looks very similar to flat-flame case... but again note $1/r$ terms vs. x in flat-flame case, plus Pe and S are unknowns (since mass flux and $Y_{F,d}$ are unknown) (and of course flame location r_f is unknown)

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Droplet combustion

- As with flat flame, energy balance at flame sheet is

$$\begin{aligned}
 -Q_R \rho D_F \frac{dY_F}{d\tilde{r}} &= k \frac{dT}{d\tilde{r}} \Big|_{\tilde{r}=\tilde{r}_{f-}} - k \frac{dT}{d\tilde{r}} \Big|_{\tilde{r}=\tilde{r}_{f+}} \Rightarrow \\
 -Q_R \rho D_F \frac{PeLe_F}{\tilde{r}_f^2} \frac{Y_{F,d}}{e^{-PeLe_F(1-1/\tilde{r}_f)} - 1} &= k \frac{Pe}{\tilde{r}_f^2} \frac{(T_f - T_d)}{1 - e^{-Pe(1-1/\tilde{r}_f)}} + k \frac{Pe}{\tilde{r}_f^2} \frac{(T_f - T_\infty)}{e^{Pe/\tilde{r}_f} - 1} \\
 -Q_R \rho D_F \frac{k}{\rho C_p D_F} \frac{Y_{F,d}}{e^{-PeLe_F(1-1/\tilde{r}_f)} - 1} &= k \frac{(T_f - T_d)}{1 - e^{-Pe(1-1/\tilde{r}_f)}} + k \frac{(T_f - T_\infty)}{e^{Pe/\tilde{r}_f} - 1} \\
 \frac{Y_{F,d} Q_R / C_p}{1 - e^{-PeLe_F(1-1/\tilde{r}_f)}} &= \frac{(T_f - T_d)}{1 - e^{-Pe(1-1/\tilde{r}_f)}} + \frac{(T_f - T_\infty)}{e^{Pe/\tilde{r}_f} - 1} \quad (\text{Eq. 2})
 \end{aligned}$$

Again looks similar to flat-flame case...

Droplet combustion

- New constraint #1 - conductive heat flux to droplet surface = enthalpy needed to vaporize the mass flux of fuel (L_v = enthalpy of vaporization at droplet temperature)

$$\begin{aligned}
 k(4\pi r_d^2) \frac{dT}{dr} \Big|_{\tilde{r}=1} &= \dot{m} L_v \Rightarrow \frac{dT}{d\tilde{r}} \Big|_{\tilde{r}=1} = \frac{\dot{m} C_p}{4\pi k r_d} \frac{L_v}{C_p} = Pe \frac{L_v}{C_p} \\
 \Rightarrow Pe \frac{T_f - T_d}{e^{Pe(1-1/\tilde{r}_f)} - 1} &= Pe \frac{L_v}{C_p} \Rightarrow e^{Pe(1-1/\tilde{r}_f)} = 1 + \frac{C_p (T_f - T_d)}{L_v} \quad (\text{Eq. 3})
 \end{aligned}$$

- New constraint #2 - mass balance at droplet surface: mass flow from droplet into gas (fuel only) = rate of fuel convected into gas + rate of fuel diffused into gas (fuel mass fraction at droplet surface ($Y_{F,d}$) cannot be 1)

$$\begin{aligned}
 \dot{m} &= -\rho D_F A \frac{dY_F}{dr} \Big|_{r=r_d} + \dot{m} Y_{F,d} \Rightarrow \frac{\dot{m} C_p}{4\pi r_d k} \frac{k}{\rho C_p D_F} (1 - Y_{F,d}) = -\frac{dY_F}{d\tilde{r}} \Big|_{\tilde{r}=1} \\
 \Rightarrow PeLe_F (1 - Y_{F,d}) &= PeLe_F \frac{Y_{F,d}}{e^{-PeLe_F(1-1/\tilde{r}_f)} - 1} \Rightarrow e^{PeLe_F(1-1/\tilde{r}_f)} - 1 = \frac{Y_{F,d}}{1 - Y_{F,d}} \\
 \Rightarrow Y_{F,d} &= 1 - e^{-PeLe_F(1-1/\tilde{r}_f)} \quad (\text{Eq. 4})
 \end{aligned}$$

Droplet combustion

- 4 equations for 4 unknowns; note $Y_{f,d}/S$ will be isolated because neither $Y_{f,d}$ nor S are known but $Y_{F,d}/S = (v_F M_F Y_{ox,\infty}) / (v_{ox} M_{ox})$ (stoichiometric mass ratio of air to pure fuel) contains only known properties

$$\text{Eq. 1: } e^{Pe Le_{ox} (1/\bar{r}_f - 1)} + S e^{Pe Le_{ox} \bar{r}_f} = 1 + S; \text{ Eq. 2: } \frac{Y_{F,d} Q_R / C_P}{1 - e^{-Pe Le_{ox} (1/\bar{r}_f - 1)}} = \frac{(T_f - T_d)}{1 - e^{-Pe (1/\bar{r}_f)}} + \frac{(T_f - T_\infty)}{e^{Pe \bar{r}_f} - 1}$$

$$\text{Eq. 3: } e^{Pe (1/\bar{r}_f)} = 1 + \frac{C_P (T_f - T_d)}{L_v}; \text{ Eq. 4: } Y_{F,d} = 1 - e^{-Pe Le_{ox} (1/\bar{r}_f)}$$

$$\text{Eq. 1} \Rightarrow Y_{F,d} = \left(\frac{Y_{F,d}}{S} \right) \frac{1 - e^{Pe Le_{ox} (1/\bar{r}_f - 1)}}{e^{Pe Le_{ox} \bar{r}_f} - 1} \text{ or } \frac{Y_{F,d}}{1 - e^{Pe Le_{ox} (1/\bar{r}_f - 1)}} = \left(\frac{Y_{F,d}}{S} \right) \frac{1}{e^{Pe Le_{ox} \bar{r}_f} - 1} \text{ (Eq. A)}$$

$$\text{Eq. A} + \text{Eq. 4} \Rightarrow \left(\frac{Y_{F,d}}{S} \right) \frac{1 - e^{Pe Le_{ox} (1/\bar{r}_f - 1)}}{e^{Pe Le_{ox} \bar{r}_f} - 1} = 1 - e^{-Pe Le_{ox} (1/\bar{r}_f)} \Rightarrow e^{Pe \bar{r}_f} = \left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} \text{ (Eq. B)}$$

$$\text{Eq. B} + \text{Eq. 2} + \text{Eq. 3} + \text{Eq. 4} \Rightarrow \frac{Q_R}{C_P} = \frac{(T_f - T_d)}{1 - \frac{L_v}{C_P (T_f - T_d)} + L_v} + \frac{(T_f - T_\infty)}{\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} - 1}$$

$$\Rightarrow \frac{Q_R}{C_P} = (T_f - T_d) + \frac{L_v}{C_P} + \frac{(T_f - T_\infty)}{\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} - 1} \Rightarrow T_f = \frac{\left(\frac{Q_R - L_v}{C_P} + T_d \right) \left(\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} - 1 \right) + T_\infty}{\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}}} \text{ (Eq. C)}$$

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Droplet combustion

$$\text{Eq. 3} \Rightarrow e^{Pe} = \frac{C_P (T_f - T_d) + L_v}{L_v} e^{Pe \bar{r}_f}$$

$$+ \text{Eq. B} + \text{Eq. C} \Rightarrow e^{Pe} = \frac{C_P \left(\frac{\left(\frac{Q_R - L_v}{C_P} + T_d \right) \left(\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} - 1 \right) + T_\infty}{\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}}} - T_d \right) + L_v}{L_v} \left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}}$$

$$\Rightarrow Pe = \ln(1 + B); B \equiv \frac{Q_R \left(\left(1 + (Y_{F,d}/S) \right)^{1/Le_{ox}} - 1 \right) + C_P (T_\infty - T_d)}{L_v} \text{ (B is called the "Transfer Number")}$$

$$\text{Note for } Le_{ox} = 1, B \equiv \frac{Q_R (Y_{F,d}/S) + C_P (T_\infty - T_d)}{L_v}, T_f = \frac{\left(\frac{Q_R - L_v}{C_P} + T_d \right) (Y_{F,d}/S) + T_\infty}{1 + (Y_{F,d}/S)}$$

$$\text{and for } (Y_{F,d}/S) \ll 1, B \approx \frac{Q_R (Y_{F,d}/S) / Le_{ox} + C_P (T_\infty - T_d)}{L_v}, T_f = \frac{\left(\frac{Q_R - L_v}{C_P} + T_d \right) \left((Y_{F,d}/S) / Le_{ox} \right) + T_\infty}{1 + (Y_{F,d}/S) / Le_{ox}}$$

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Droplet combustion

- So finally we can calculate the droplet burning rate using Pe in terms of known properties

$$Pe \equiv \frac{\dot{m}C_p}{4\pi kr_d} = \ln(1+B), \dot{m} = \rho_d u_d A_d = \rho_d \frac{dr_d}{dt} 4\pi r_d^2 \Rightarrow \rho_d \frac{dr_d}{dt} 4\pi r_d^2 \frac{C_p}{4\pi kr_d} = \ln(1+B)$$

$$\Rightarrow r_d \frac{dr_d}{dt} = \frac{k}{\rho_d C_p} \ln(1+B) \Rightarrow r_d dr_d = \frac{k}{\rho_d C_p} \ln(1+B) dt \Rightarrow \frac{r_d^2}{2} = \frac{d^2}{8} = \frac{k}{\rho_d C_p} \ln(1+B) t + C;$$

$$\text{Initial condition } d_d = d_d(0) \text{ at } t = 0 \Rightarrow d_d^2(0) - d_d^2(t) = \frac{8k}{\rho_d C_p} \ln(1+B) t = Kt$$

K is called the "burning rate constant" (typically 0.5 mm²/s)

- What about r_f and $Y_{F,d}$?

$$\tilde{r}_f = Pe \ln(1 + (Y_{F,d}/S))^{-1/Le_{ox}} \Rightarrow \tilde{r}_f = \frac{r_f}{r_d} = \frac{d_f}{d_d} = \frac{Le_{ox} \ln(1+B)}{\ln(1 + (Y_{F,d}/S))}$$

$$Y_{F,d} = 1 - e^{-Pe Le_F (1 - 1/\tilde{r}_f)} = 1 - e^{-Pe Le_F} e^{-Pe Le_F / \tilde{r}_f} = 1 - \frac{(1 + (Y_{F,d}/S))^{Le_F/Le_{ox}}}{(1+B)^{Le_F}}$$

$$\text{For } Le_F = Le_{ox} = 1, Y_{F,d} = \frac{B - (Y_{F,d}/S)}{1+B}$$

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Droplet combustion - comments

- $(8k/\rho_d C_p) \ln(1+B)$ is called the **burning rate constant** – units length²/time
- $k/\rho_d C_p$ is NOT the thermal diffusivity because ρ_d is the **droplet (liquid) density**, not gas density!
- B is called the **Transfer Number** – ratio of enthalpy generated by combustion to enthalpy need to vaporize fuel; typical values for hydrocarbons ≈ 10 , much lower for methanol (≈ 3)
- Enthalpy release (Q_R) appears only inside a $\ln(\)$, thus changing T_f hardly affects burning rate at all - why? The more rapidly fuel is vaporized, the more rapidly the fuel vapor blows out, thus the harder it is for heat to be conducted back to the fuel surface
- In fact since you can't change k , ρ_d or C_p significantly in fuel/air combustion, only the droplet diameter affects burning time significantly (time $\sim d_d(0)^2$)
- d_f/d_d is constant and doesn't even depend on transport properties (except for Le_{O_2}), just thermodynamic properties!

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Droplet combustion - comments

- As expected, as $Y_{O_2,\infty}$ decreases (more diluted oxidizer), flame moves farther out (r_f increases) due to lower fuel flux
- Flame temperature almost same as gaseous flame with adjusted enthalpy release $Q_R - L_v$ vs. Q_R
- Since usually $Y_{F,d}/S \ll 1$ (see example), $Y_{F,d} \approx B/(1+B)$ which is generally only slightly less than 1 since generally $B \gg 1$
- Can also use this formula for \dot{m} even if no combustion (just evaporation of a cold droplet in a hot atmosphere) – set $Q_R = 0$
- Nothing in expression for Pe , T_f , r_f or $Y_{F,d}$ depends on pressure
- Le_F doesn't affect burning rate (Pe), r_f or T_f at all, only $Y_{F,d}$ due to a cancellation of Le_F in the boundary conditions at $r = r_f$ and $r = r_d$
- As a result, there are "simple" closed-form solutions even for $Le \neq 1$, whereas for the 1D planar unstretched flame and the 1D counterflow, different types of boundary conditions exist at the flame sheet (flux matching) and reactant supply boundary (specified value) thus closed-form solutions for $Le \neq 1$ do not exist

Droplet combustion - comments

- For decreasing Le_{O_2}
 - B (thus Pe) increases, but not much because of $\ln(1+B)$ term
 - r_f decreases because of Le_{O_2} term; increasing B inside $\ln()$ term has less effect
 - T_f increases because of $(1/Le_{O_2})$ exponent
- Actually there is a 5th equation since T_d and $Y_{F,d}$ are not dependent – a liquid-vapor equilibrium exists, typically modeled via the Clausius-Clapeyron relation

$$X_{F,d} = \exp\left[\frac{L_v}{\mathcal{R}}\left(\frac{1}{T_b} - \frac{1}{T_d}\right)\right]; T_b = \text{boiling point of pure liquid at ambient pressure}$$

$$X_{F,d} = \text{mole fraction of fuel at droplet surface} = Y_{F,d} \frac{M_F/M_{inert}}{1 + Y_{F,d}(M_F/M_{inert} - 1)}$$

... but for typical fuel-air combustion, effect on burning rate constant K is small because $Y_{F,d}$ is close to 1 (but must be < 1).

Droplet combustion

- Comment on T and Y_{ox} profiles for $r \rightarrow \infty$

$$\text{As } r \rightarrow \infty: T(\tilde{r}) = \frac{(T_f - T_\infty e^{-Pe/\tilde{r}}) - (T_f - T_\infty)e^{-Pe/\tilde{r}}}{1 - e^{-Pe/\tilde{r}}} \rightarrow \frac{(T_f - T_\infty e^{-Pe/\tilde{r}}) - (T_f - T_\infty)(1 - Pe/\tilde{r})}{1 - e^{-Pe/\tilde{r}}}$$

$$= T_\infty + \frac{T_f - T_\infty}{1 - e^{-Pe/\tilde{r}}} \frac{Pe}{\tilde{r}} \sim \frac{1}{\tilde{r}}$$

$$\text{Also since typically } \tilde{r}_f \gg 1, T(\tilde{r}) \rightarrow T_\infty + \frac{T_f - T_\infty}{1 - (Pe/\tilde{r}_f)} \frac{Pe}{\tilde{r}} = T_\infty + (T_f - T_\infty) \frac{\tilde{r}_f}{\tilde{r}}$$

$$\text{Similarly } Y_{ox}(\tilde{r}) = Y_{ox,\infty} \left(1 - \frac{1}{1 - e^{-PeLe_{ox}/\tilde{r}}} \frac{PeLe_{ox}}{\tilde{r}} \right) \text{ and for } \tilde{r}_f \gg 1, Y_{ox}(\tilde{r}) \rightarrow Y_{ox,\infty} \left(1 - \frac{\tilde{r}_f}{\tilde{r}} \right)$$

- This is identical to pure diffusion in spherical geometry:

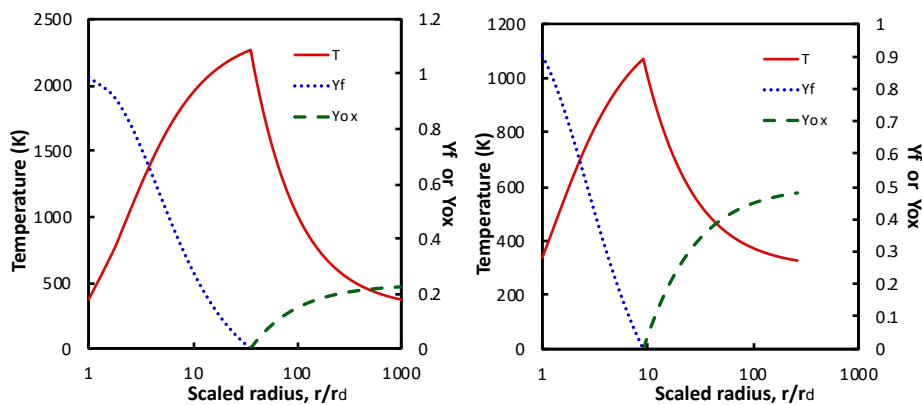
$$\frac{d}{dr} \left(r^2 \frac{dT}{dr} \right) = 0 \Rightarrow T(r) = C_1 + \frac{C_2}{r}; \quad \frac{d}{dr} \left(r^2 \frac{dY_{ox}}{dr} \right) = 0 \Rightarrow Y_{ox}(r) = C_1 + \frac{C_2}{r}$$

$$\text{BCs } T = T_f \text{ at } r = r_f, T = T_\infty \text{ at } r = \infty \Rightarrow T(r) = T_\infty + (T_f - T_\infty) \frac{r_f}{r}$$

$$\text{BCs } Y_{ox} = 0 \text{ at } r = r_f, Y_{ox} = Y_{ox,\infty} \text{ at } r = \infty \Rightarrow Y_{ox}(r) = Y_{ox,\infty} \left(1 - \frac{r_f}{r} \right)$$

so diffusion dominates convection at large r

Droplet combustion



n-C₇H₁₆ - air

CH₃OH - O₂/He

Droplet combustion

- Example for typical fuel (heptane, C_7H_{16}) in air (assuming $Le_F = Le_{O_2} = 1$, but again Le_F affects only $Y_{F,d}$)

$$d_d^2(0) - d_d^2(t) = \frac{8k}{\rho_d C_p} \ln(1+B)t; B = \frac{Q_R(Y_{F,d}/S) + C_p(T_\infty - T_d)}{L_v}; \frac{Y_{F,d}}{S} = Y_{\infty, \infty} \frac{v_F M_F}{v_{\infty, \infty} M_{\infty}} = 0.233 \frac{1(100)}{11(32)} = 0.0662$$

$$B = \frac{(4.46 \times 10^7 J/kg)(0.0662) + (1400 J/kgK)(298K - 371.5K)}{3.18 \times 10^5 J/kg} = 8.96$$

$$\text{Burning rate constant } K = \frac{8k}{\rho_d C_p} \ln(1+B) = \frac{8(0.026 W/mK)}{(680 kg/m^3)(1400 J/kgK)} \ln(1+8.96)$$

$$= 5.0 \times 10^{-7} m^2/s = 0.50 mm^2/s$$

$$\text{Flame diameter } \frac{d_f}{d_d} = \frac{\ln(1+B)}{\ln(1+(Y_{F,d}/S))} = \frac{\ln(1+8.96)}{\ln(1+0.0662)} = 35.9$$

$$\text{Flame temperature } T_f = \frac{(Q_R - L_v)/C_p + T_d + (S/Y_{F,d})T_\infty}{1 + S/Y_{F,d}}$$

$$= \frac{(4.46 \times 10^7 - 3.18 \times 10^5 J/kg)/(1400 J/kgK) + 371.5K + (1/0.0662)(298K)}{1 + 1/0.0662} = 2267K$$

$$\text{Fuel mass fraction at droplet surface } Y_{F,d} = \frac{B - (Y_{F,d}/S)}{1+B} = \frac{8.96 - 0.0662}{1+8.96} = 0.893$$

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Droplet combustion

- The d^2 -law assumes no buoyant or forced convection, but in most applications there is likely to be significant flow; one relation for the effect of flow on burning rate is

$$[d(0)]^2 - [d(t)]^2 = Kt; K = \frac{4 Nu k}{\rho_d C_p} \ln(1+B); Nu = 2 + \frac{0.555 Re_d^{1/2} Pr^{1/3}}{[1 + 1.232/(Re_d Pr^{4/3})]^{1/2}}$$

Re_d = Droplet Reynolds number = $ud(t)/\nu$

Nu = Nusselt number based on droplet diameter

u = droplet velocity relative to gas

Pr = Prandtl number = ν/α

ν = kinematic viscosity

α = thermal diffusivity = $k/\rho C_p$

- Reduces to the previous result for $u = 0$ (thus $Re = 0$)

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Summary

- The structure of premixed and nonpremixed 1D laminar flames is determined by
 - Balance between conduction & convection outside reaction zones
 - Matching of reactant consumption within reaction zone in stoichiometric proportions to flux of reactants into reaction zone
 - Matching of thermal enthalpy release within reaction zone to diffusion (conduction) of heat away from reaction zone
- Nominally, flame temperature of premixed flames is determined by thermodynamics alone
- Flame temperature of nonpremixed flames is very dependent on convective (Peclet #) and diffusive (Lewis number) effects, but for usual situation of highly diluted O₂ (*i.e.*, air) ($S \gg 1$) with $Le_{O_2} \approx 1$, these effects are minimal

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