< Premixed Laminar Flame >

Flame Zone
$\Big($
Preheat zone
Reaction zone : intermediate species production
Oxidation zon : intermediate species are oxidized
  to produce stable products.

fuel rxn zone

fuel (CH4)

δ

Temperature

CO.

H_2

Preheat $\longrightarrow$ $\longleftarrow$ Oxidation zone
zone

- Global chemical model.

$\rightarrow$ two-step irreversible rxn. $\rightarrow$ Thee-zone model

$$CH_4 + O_2 \xrightarrow{\;I\;} Intermediates\,(CO, H_2) \xrightarrow{\;II\;} products$$
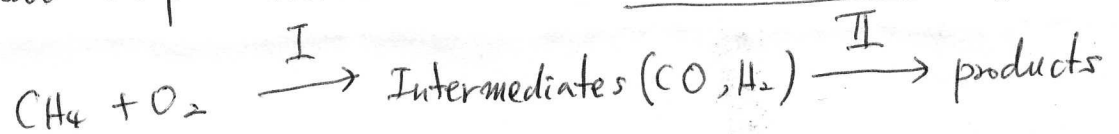
$*$ rxn (II) is faster than rxn (I)
  $\Rightarrow$ quasi-steady state for intermediates.

$\rightarrow$ one-step irreversible rxn $\Rightarrow$ Two-zone model.

$$CH_4 + O_2 \xrightarrow{\;I\;} products.$$

$*$ δ (thickness of rxn zone) is negligibly small.

$\Rightarrow$ The two different models for flame structure
  to obtain $\boxed{\text{premixed laminar flame speed}}$

Two - zone model

- Consv. of mass $(\rho u = \dot{m}'' = const.)$
- Consv. of energy $(h = const.)$
- species equations.
- ideal gas equation of state $\underline{(p = const.)}$

  $\uparrow$

  proven previously.

$$\text{Lewis \# } (Le) \equiv \frac{\alpha}{D}$$

$$\alpha = \frac{\lambda}{\rho C_p} \quad \leftarrow \text{themal conductivity.} \quad = \text{themal diffusivity.}$$

when $\underline{Le = 1}$. energy equation

$$\Rightarrow \nabla \cdot (\rho \vec{v} h_{sens} - \rho D \nabla h_{sens}) = -RR''' (\Delta H_R)$$

Recall Shvab-Zeldovich transformation

$$\nabla \cdot [\rho \vec{v} \, \eta_T - \rho D \nabla \eta_T] = RR'''$$

$$\eta_T \equiv \frac{h_{sens}}{-\Delta H_R}.$$

* Let's assume 1-D phenomena along x-cordinate

$$\vec{v} = u \hat{z}$$

$$L(\eta) = \rho u \frac{d\eta}{dx} - \frac{d}{dx}(\rho D \cdot \frac{d\eta}{dx}) = RR'''$$

$$\Rightarrow RR'''(-\Delta H_R) = \rho u \frac{dh_{sens}}{dx} - \frac{d}{dx}(\rho D \frac{dh_{sens}}{dx})$$

for ideal gas, $h_{sens} = \int_{T_{ref}}^{T} C_p(T) dt$

$$dh = C_p(T) dT \quad \& \quad \frac{dh}{dT} = C_p(T)$$

$$\therefore \frac{dh}{dT} \cdot \frac{dT}{dx} = \frac{dh}{dx} = \underline{C_p(T) \frac{dT}{dx}} \quad //$$

$$\therefore \rho u \, C_p \frac{dT}{dx} - \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) = RR_{fuel}''' \, (\Delta H_c) \; (= RR'''(-\Delta H_R))$$

heat of combustion.

$$Le = 1 = \frac{\alpha}{D} = \frac{\lambda}{\rho C_p D} \qquad = -\Delta H_R / \text{fuel mass.}$$
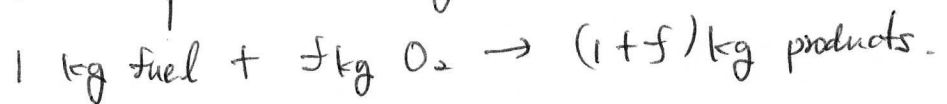
$$\therefore \lambda = \rho C_p D$$

B.C.

$x \rightarrow -\infty$: unburned gas , $T = T_u$, $\frac{dT}{dx} = 0$

$x \rightarrow \infty$: burned gas , $T = T_b$, $\frac{dT}{dx} = 0$
    $(= T_{ad})$

✳ one-step irreversible global rxn.

  1 kg fuel + f kg O_2 → $(1+f)$ kg products.

$$RR_{fuel}''' \; (\text{kg fuel} / \text{volume} \cdot \text{time}) = -A \, \rho_{fuel}^a \, \rho_{O_2}^b \, \exp\left(-\frac{E_{ov}}{\hat{R}T}\right)$$
                    m^3 sec.
                         destruction (consumption) of fuel

a, b : orders of the global rxn for fuel and oxygen.

E_{ov} : overall activation energy.

✳ Critical Assumptions for two-zone model.
○ rxn zone is much thinner than preheat zone
○ rxns in the preheat zone are negligible $(RR_{preheat}''' = 0)$

⇒ Preheat zone.
$$\int \left(\rho u \, C_p \frac{dT}{dx} - \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) = 0 \right)$$

$= \rho_u S_u$
    ↑
flame speed.
              $\Rightarrow \rho_u S_u \langle C_p \rangle T - \lambda \frac{dT}{dx} = \text{constant.}$

$\Rightarrow T = T_u, \frac{dT}{dx} = 0$, on the boundary of preheat zone for cold gas.

$$\therefore \rho_u S_u \langle c_p \rangle T_u = \text{constant.}$$

$$\Rightarrow \rho_u S_u \langle c_p \rangle T - \lambda \frac{dT}{dx} = \rho_u S_u \langle c_p \rangle T_u$$

$$\rho_u S_u \langle c_p \rangle (T - T_u) = \lambda \frac{dT}{dx}$$

at $x = x_i$ on the boundary between preheat & rxn zones.

$$\lambda \frac{dT}{dx}\Big|_{x=x_i} = \rho_u S_u \langle c_p \rangle (T_i - T_u)$$

* __Conductive__ heat transfer from (T_i) to (T_u)

⟳ rxn zone

* T_i is slightly lower than T_b.

$$\therefore \frac{dT}{dx} \ll \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right)$$

$$\therefore -\frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) = RR''_{fuel}(\Delta H_c)$$

→ Integrate from $x = x_i$ to $x = \infty$.

$$\left(\begin{array}{c} T = T_i \\ \frac{dT}{dx} = \frac{dT}{dx}\Big|_{x_i} \end{array} \right. \qquad \left(\begin{array}{c} T = T_b \\ \frac{dT}{dx} = 0 \end{array}\right.$$
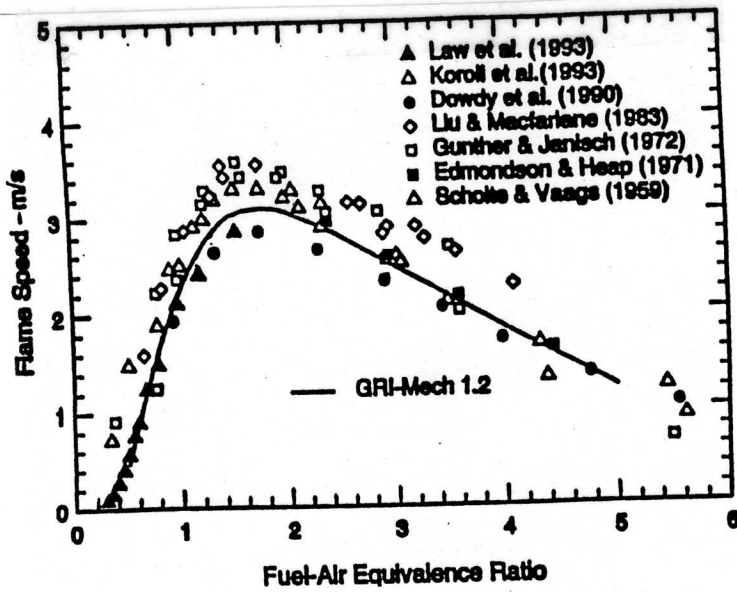
$$\therefore \lambda \frac{dT}{dx}\Big|_{x_i} = \left(2 \Delta H_c \int_{T_i}^{T_b} \langle \lambda \rangle RR''_{fuel}\, dT\right)^{1/2}$$

$$= \rho_u S_u \langle c_p \rangle \cdot (T_i - T_u)$$

$$S_u = \left[\left(\underbrace{\frac{\langle \lambda \rangle}{\rho_u \langle c_p \rangle}}_{\langle \alpha \rangle}\right)\left(\frac{2 \Delta H_c}{\rho_u \langle c_p \rangle (T_i - T_u)}\right) \cdot \left(\frac{1}{T_i - T_u}\right) \cdot \underbrace{\int_{T_i}^{T_b} RR''_{fuel}\, dT}_{\equiv \langle RR''_{fuel}\rangle}\right]^{1/2}$$

⟨ Premixed Laminar Flame ⟩

* Laminar flame speed is our interest.

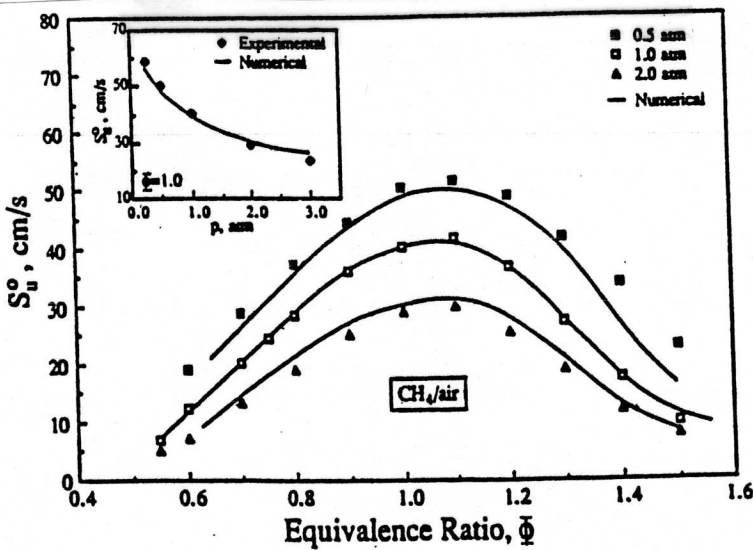Laminar flame speeds for H_2-air at atmospheric pressure.

- S_u is max at $\phi \cong 1.7$ for H_2

- for alkanes ($C_n H_{2n+2}$) S_u is max at $\phi = 1.1$.

  alkene ($C_n H_{2n}$)
  max S_u at $\phi = 1.2$
  alkyne ($C_n H_{2n-2}$)
  max S_u at $\phi = 1.4$

* Hydrogen flame speed as a function of equivalence ratio.

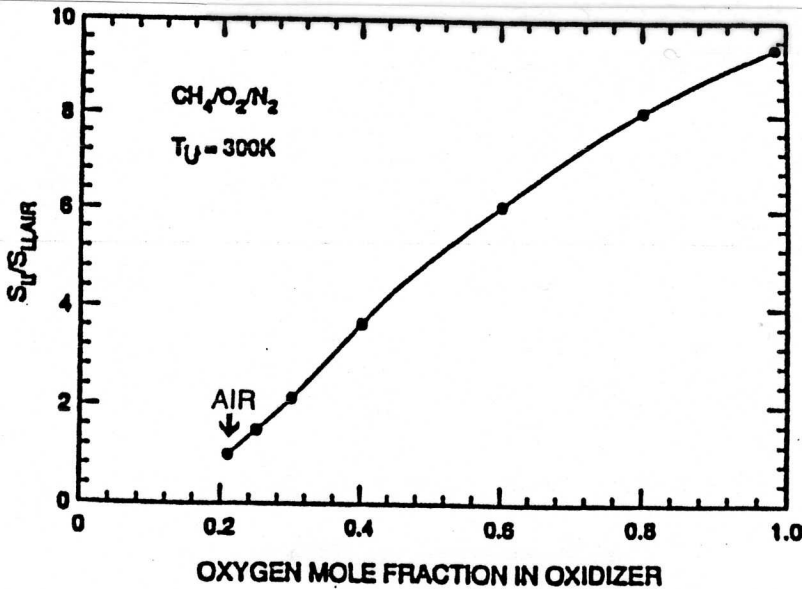Laminar flame speeds for CH_4-air. The inset shows the pressure-
of the stoichiometric flame speed. The solid lines are calculated f
using PREMIX and a detailed reaction mechanism. (Law et al.,

* pressure dependence of methane/air premixed flame.

  Recall that for hydrocarbons $(a+b < 2)$
  $$P \uparrow \implies S_u \downarrow$$

- at 1 atm, max alkane S_u $\simeq 40$ cm/s
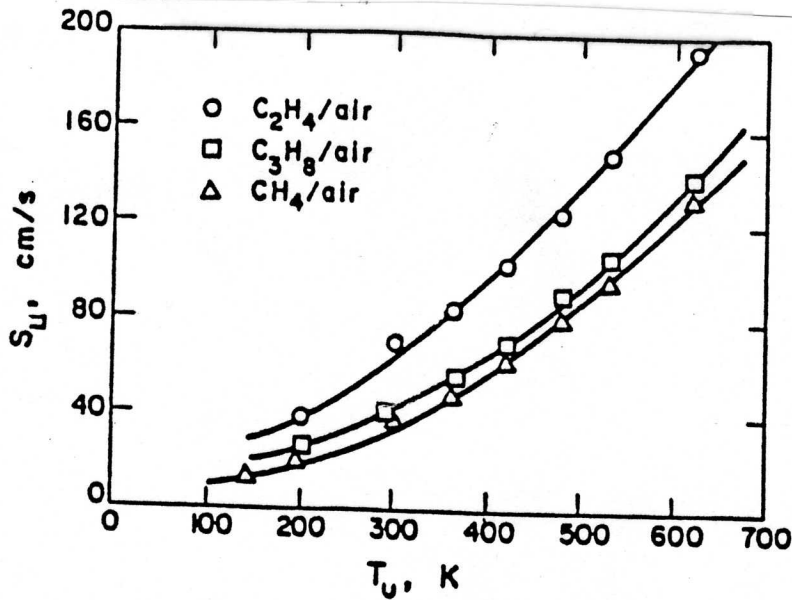
Measured variation of laminar flame speed for stoichiometric hydrocarbon-air mixtures with reactant temperature at atmospheric pressure.
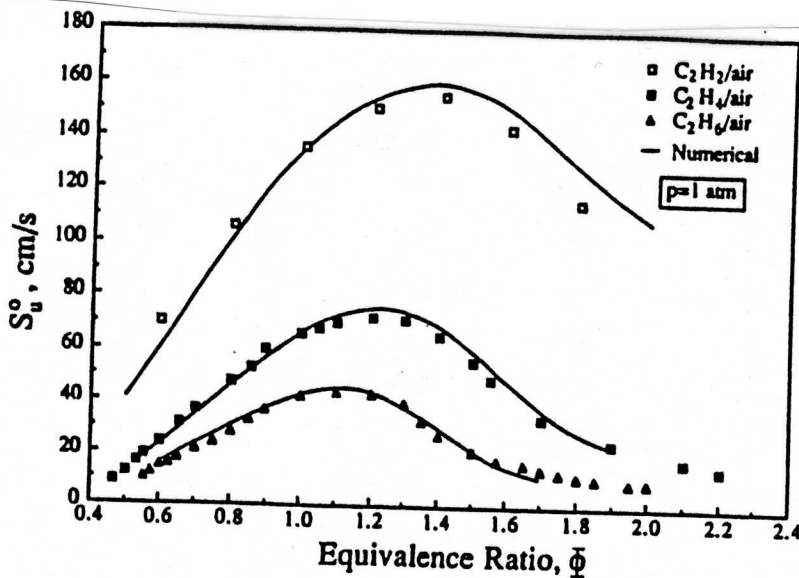
✻ Influence of un burned gas temperature.

∴ $T_u \uparrow \rightarrow T_b \uparrow$ (energy conservation)

Measured laminar flame speeds for stoichiometric CH_4-O_2-N_2 mixtures at atmospheric pressure (Lewis and von Elbe, 1961).
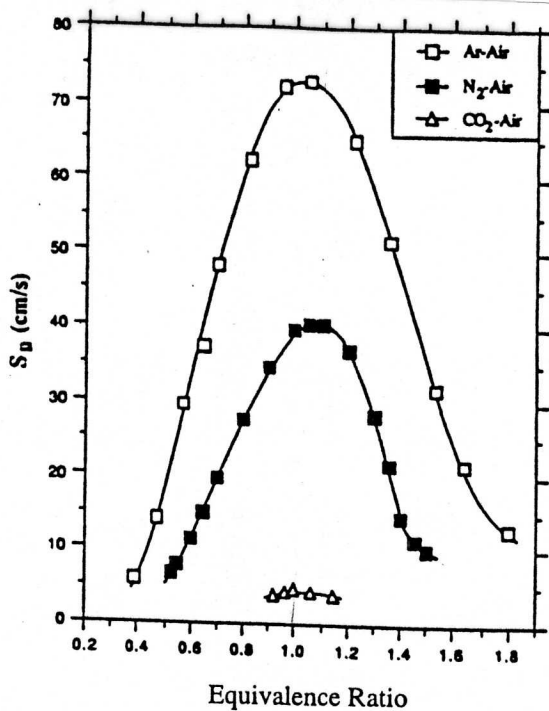
✻ Influence of oxygen mole fraction. $X_{O_2} \uparrow \Rightarrow S_u \uparrow$

∴ $X_{O_2} \uparrow \Rightarrow \rho_{O_2} \uparrow \Rightarrow R\dot{R}'' \uparrow$

Laminar flame speeds for C_2-hydrocarbon-air mixtures at atmospheric pressure. The solid lines are calculated flame speeds using PREMIX and detailed reaction mechanisms (Law et al., 1990).

* Flame speed dependence on fuel species, C_2H_m.

Measured laminar flame speeds for CH_4-"air" mixtures for three diluents - N_2, Ar, and CO_2 at atmospheric pressure (Law et al., 1988).

* Influence of diluent.

Oxidizer combination

$$\begin{cases} 20\% \ O_2 \ + \ 80\% \ Ar \\ 20\% \ O_2 \ + \ 80\% \ N_2 \\ 20\% \ O_2 \ + \ 80\% \ CO_2 \end{cases}$$

$$\begin{cases} C_{p_{Ar}} = 20.8 \ J/mol \cdot K. \\ C_{p_{N_2}} = 29.1 \ J/mol \cdot K \\ C_{p_{CO_2}} = 36.9 \ J/mol \cdot K. \end{cases}$$
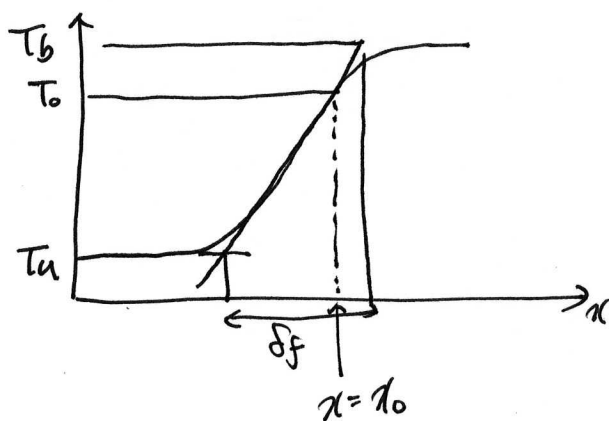
$\Rightarrow$ same heat energy with different Heat Capacity.

$\Rightarrow T_b$ decreases as C_p increases

Recall: $T_b \downarrow \Rightarrow S_u \downarrow$

◎ Flame thickness.

* Temperature/concentration gradients in flame depend on flame thickness
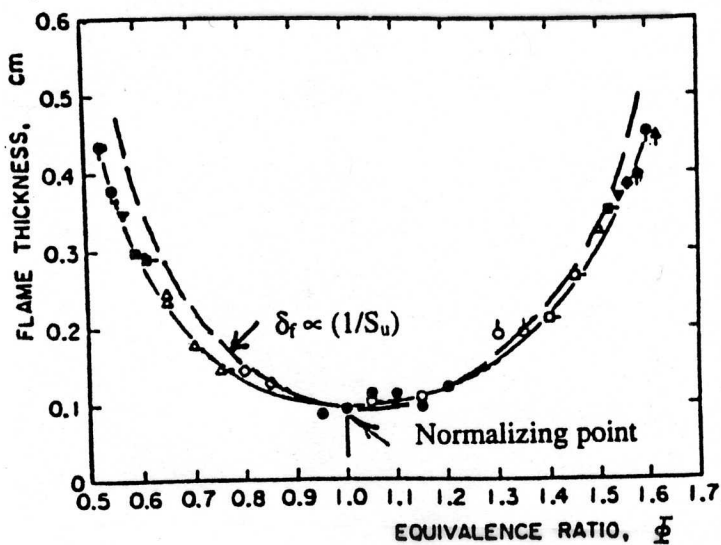

* energy balance

$$\rho_u S_u \langle C_p \rangle (T_0 - T_u) = \lambda \frac{dT}{dx}\Big|_{x=x_0} = \lambda \frac{T_b - T_u}{\delta_f}$$

Heat absorbed ↑
in preheat zone.

↑ heat flux from rxn zone

○ $T_0 \approx T_b$ for large activation energy.

$$\delta_f \approx \frac{\lambda}{\rho_u \langle C_p \rangle} \cdot \frac{1}{S_u} = \frac{\langle \alpha \rangle}{S_u}$$

$\langle \alpha \rangle$ is a weak function of stoichiometry.

← for methane/air flame.

In a two-zone model

$$\delta_r \ll \delta_{ph}$$

↑   ↑

rxn zone   preheat zone.

$$\frac{\delta_r}{\delta_{ph}} = \frac{T_b - T_o}{T_o - T_u} \approx \frac{T_b - T_o}{T_b - T_u}$$

$$T_b - T_o \approx \frac{RR_{fuel}'''(T_b)}{\dfrac{d(RR_{fuel}'''(T_b))}{dT}} = \frac{\hat{R} T_b^2}{E_{50}}$$

$$\therefore \frac{\delta_r}{\delta_{ph}} \approx \frac{\hat{R} T_b^2}{E_{50}(T_b - T_u)} \equiv \frac{1}{\beta} \nwarrow \text{Zeldovich \#}$$

and $\quad \delta_f \approx \dfrac{\langle \alpha \rangle}{S_u} \quad . \quad S_u \propto P^{\frac{a+b-2}{2}}$

$$\langle \alpha \rangle \propto \frac{T^n}{P}$$

$$\therefore \underline{\delta_f \propto P^{-\frac{a+b}{2}}}_{//} \qquad a, b \text{ are empirical global kinetics parameters.}$$

$$\underline{\Rightarrow P \uparrow \Rightarrow \delta_f \downarrow}_{//}$$