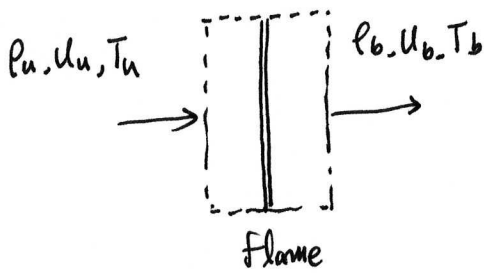


# Laminar Premixed Flame II

• Two-zone model.

\* global energy balance



$$\dot{m}_f'' (-\Delta H_c) = \dot{m}'' \langle C_p \rangle (T_b - T_u)$$

$\uparrow$  combustion energy                       $\uparrow$  sensible enthalpy increase.

$$\frac{\dot{m}_f''}{\dot{m}''} = Y_{f_0} \quad \therefore Y_{f_0} (-\Delta H_c) = \langle C_p \rangle (T_b - T_u)$$

$$\Rightarrow \frac{-\Delta H_c}{\rho_u \langle C_p \rangle (T_b - T_u)} = \frac{1}{Y_{f_0} \rho_u}$$

previously,  $S_u = \left\{ \langle \alpha \rangle \left( \frac{2\Delta H_c}{\rho_u \langle C_p \rangle (T_b - T_u)} \right) \left( \frac{1}{T_b - T_u} \right) \left( \int_{T_u}^{T_b} RR_{fuel}'' dT \right) \right\}^{1/2}$

$= -2 \frac{\langle \alpha \rangle}{Y_{f_0} \rho_u} = \langle RR_{fuel}'' \rangle$

$$\therefore S_u = \left( \frac{-2\langle \alpha \rangle}{Y_{f_0} \rho_u} \langle RR_{fuel}'' \rangle \right)^{1/2}$$

$\leftarrow$  diffusive transport  
 $\uparrow$  Reaction kinetics, approximated  $RR_{fuel}''$  at  $T_b$

$$\alpha \propto \frac{T^n}{p}$$

$n = \frac{3}{2}$  for monatomic gases  
 $= 1.8$  non-condensable diatomic & triatomic gases

$\therefore$  Mostly, rxn occurs in the high temperature condition over  $T_0$  (cross over temperature)  
 $T_0 \approx T_b$  for high activation energy.

Recall,  $RR_{fuel}''' = -A \rho_{fuel}^a \rho_{O_2}^b \exp\left(-\frac{\bar{E}_{O_2}}{\hat{R}T}\right)$

⊙ Dependence of  $S_u$  on pressure & temperature

$$S_u \propto \left( \frac{\langle a \rangle}{\rho_{fuel}} \langle RR_{fuel}''' \rangle \right)^{\frac{1}{2}} \propto \frac{T^{\frac{1}{2}}}{\rho^{\frac{1}{2}}} \cdot \rho^{\frac{a}{2}} \cdot \rho^{\frac{b}{2}} \cdot \exp\left(-\frac{\bar{E}_{O_2}}{2\hat{R}T_b}\right)$$

$\rho_{fuel} \propto \rho$        $\rho_{O_2} \propto \rho$

$$\therefore S_u = \text{constant} \times \underbrace{\rho^{\frac{a+b-2}{2}}}_{\text{only pressure term.}} f(T_u, T_b) \exp\left(-\frac{\bar{E}_{O_2}}{2\hat{R}T_b}\right)$$

$\uparrow$  temperature influence on  $\alpha$  &  $Y_{f_0}$

\* for most hydrocarbons  $a+b < 2$

$$\therefore \underline{P \uparrow \Rightarrow S_u \downarrow}$$

\* when  $\frac{\bar{E}_{O_2}}{2\hat{R}} \gg T_b$ , then temperature dependence is governed largely by  $\exp\left(-\frac{\bar{E}_{O_2}}{2\hat{R}T_b}\right)$

$$\Rightarrow \underline{T_b \uparrow} \Rightarrow S_u \uparrow$$

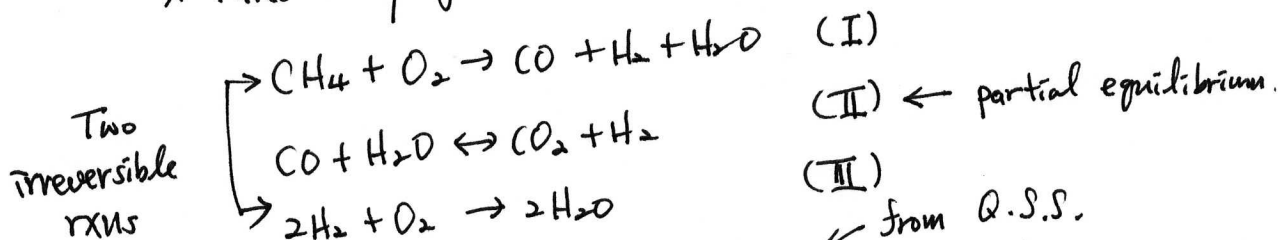
depends on ① equivalence ratio, ② oxygen mole fraction in oxidizer  
 ③ reactant temperature, ④ specific heat of diluent

◦ Three-zone model.

\* Two-step global reaction  
Thickness of the three zones.

preheat zone  $\gg$  oxidation zone  $\gg$  reaction zone (fuel oxidation zone)

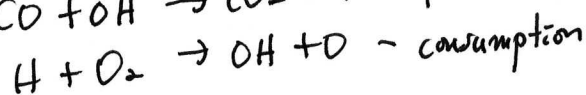
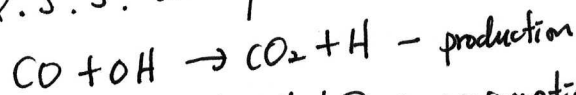
\* three-step global reaction mechanism (N. Peters, 1999)



$\Rightarrow$  Rate of (I) is governed by  $\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$

$\Rightarrow$  Rate of (III) is governed by  $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$

Q.S.S. assumption for [H]

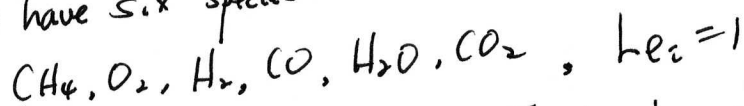


◦ In reaction zone (intermediate/fuel oxidation zone), convective flux is neglected since the thickness is very thin.

$$\therefore L(\eta_i) = -\frac{d}{dx} (\rho D_i \frac{d\eta_i}{dx}) = \sum_j \underbrace{R R_{i,j}}''$$

$\sum_j$  global rxns involving species  $i$

◦ We have six species.



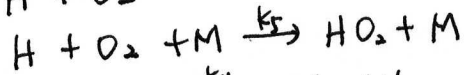
◦ Let's assume temperature =  $T_0$  in the rxn zone.

◦ In the fuel oxidation zone  $Y_f = 0$  (no fuel)  
only rxn III rate drives rxn in oxidation layer.

You can choose  $\text{H}_2$  or  $\text{CO}$  for the analysis in the oxidation layer

\* D.C.s and the PDE solution gives.

$$\frac{k_1^2(T_0) \cdot \tilde{R} T_0}{k_{11}(T_0) \cdot k_5(T_0)} = 1.5 P$$



$\Rightarrow T_0$  is a function of pressure, not  $T_u$  or diluent concentration

$$S_u^2 \propto \frac{k_1(T_0)^2}{k_{11}(T_0)} \cdot \frac{1}{X_{H_2O}^{0.5}} \cdot \frac{T_{fu}}{M_f} \cdot \frac{\lambda(T_0)}{Q_p(T_0)} \cdot \left( \frac{K_{IV}(T_0)}{1 + \alpha(T_0)} \right)^{1/2} \left( \frac{T_u}{T_0} \right)^2 \cdot \left( \frac{T_b - T_0}{T_b - T_u} \right)^4$$

$K_{IV}(T_0)$  = equilibrium constant for  $O_2 + 3H_2 \leftrightarrow 2H + 2H_2O$

$$\alpha(T_0) = \frac{[CO_2]}{[H_2O] K_{II}(T_0)}$$

\* pressure dependence of  $S_u$  is implicit through the effect of pressure on  $T$

