Solutions to selected problems in
Tutorial 1 & 2.

Tutorial 1

P3. $X_{H_2} = 0.8$, $X_{O_2} = 0.2$

$u_{H_2} = 20\ \frac{m}{s}$, $u_{O_2} = 10\ \frac{m}{s}$

Mole averaged velocity $\hat{u} = \sum_i X_i u_i = 0.8\times 20 + 0.2\times 10$
$= 18$ m/s

Mass averaged velocity $\bar{u} = \sum Y_i u_i = 0.2\times 20 + 0.8\times 10 = 12$ m/s

$$Y_i = \frac{X_i W_i}{\sum_i X_i W_i} \longrightarrow Y_{H_2} = 0.2,\ Y_{O_2} = 0.8$$

$u = \hat{u} + \hat{V} \Rightarrow \hat{V}_{H_2} = 2$ m/s, $\hat{V}_{O_2} = -8$ m/s

$u = \bar{u} + \bar{V} \Rightarrow \bar{V}_{H_2} = 8$ m/s, $\bar{V}_{O_2} = -2$ m/s

P4. $\rho_{mix} = 1.2\ kg/m^3$

→ $Y_A(x) = 0.8 - 2x$; $\Rightarrow Y_B(x) = 1 - Y_A(x)$

$D_{AB} = 5\times 10^{-5}\ m^2/s$

$$J_A = \rho Y_A V_A = \rho Y_A\left(-\frac{D_{AB}}{Y_A}\frac{dY_A}{dx}\right) = -\rho D_{AB}\frac{dY_A}{dx}$$

$$J_B = \rho Y_B V_B = -\rho D_{AB} \frac{dY_B}{dx}$$

$J_A = 12 \times 10^{-5} \frac{kg}{m^2 s}$; $J_B = -12 \times 10^{-5} \frac{kg}{m^2 s}$

$u = 0.01 \frac{m}{s}$; $F_A = \rho Y_A u + J_A = \dots = 7.32 \times 10^{-3} \frac{kg}{m^2 s}$

$F_B = \rho Y_B u + J_B = \dots = 4.68 \times 10^{-3} \frac{kg}{m^2 s}$

P5.

$$\nabla X_i = \sum_j \frac{X_i X_j}{D_{ij}} \left(\underline{V_j} - \underline{V_i} \right)$$

① Simplify $D_{ij} = D \implies D \nabla X_i = X_i \left(\underbrace{\sum_j X_j \underline{V_j}} - \underbrace{\underline{V_i}}_{\text{vector}} \right)$ — ①

② Multiply $\sum_i$ ① $* Y_i$

$$\Rightarrow D \sum_i Y_i \bar{\nabla} \ln X_i = \underbrace{\sum_j X_j V_j}$$ — ②

③ Use ② in ① $\rightarrow$ get an expression for $\underline{V_i}$

$$\underline{V_i} = \sum_k Y_k D \bar{\nabla} \ln X_k - D \bar{\nabla} \ln X_i$$

④ Write X_k in terms of Y_k $\xrightarrow{\text{simplify}}$

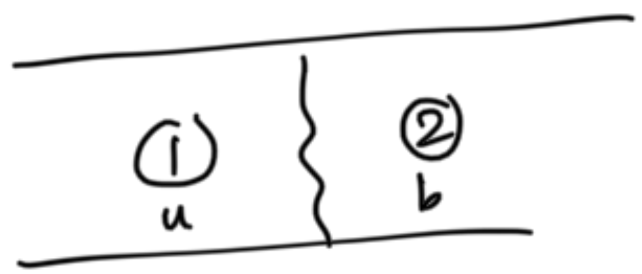
Note: $\bar{\nabla} X_k = \bar{\nabla}\left(\frac{Y_k}{W_k} W\right) = \underline{\underline{\left(\frac{W}{W_k}\bar{\nabla} Y_k\right)}} + \underline{\underline{\left(\frac{Y_k}{W_k}\bar{\nabla} W\right)}}$

$X_k = \left(\frac{Y_k}{W_k} \cdot W\right)$

$\Downarrow$ Simplify

$V_i = -D \bar{\nabla} \ln Y_i$

P6. $\displaystyle\int_{-\infty}^{\infty} \frac{dp}{dx} = -\int_{-\infty}^{\infty} \rho u \frac{du}{dx}$



$p_2 - p_1 = -(\rho u)_1 (u_2 - u_1)$ — ①

$\rho_1 u_1 = \rho_2 u_2 \Rightarrow \frac{u_2}{u_1} = \frac{\rho_1}{\rho_2} = \frac{p_1}{T_1}\frac{T_2}{p_2} = \left(\frac{T_2}{T_1}\right)\left(\frac{p_1}{p_2}\right)$ — ②

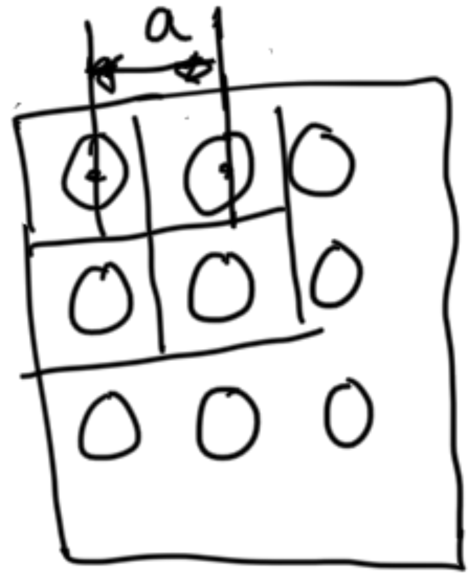
Put ② in ① $\longrightarrow$ Simplify

$u_1 = 0.4 \frac{m}{s}$; Take $\rho = 1.2 \frac{kg}{m^3}$, $\frac{T_2}{T_1} = 7$

$p_2 - p_1 = -1.5$ Pa (Check!!)

↳ My number may be incorrect

P8.



Find :

→ No. of holes per unit area ✓

→ Diameter of circular holes ✓

→ Hole-centerline spacing

$$\rightarrow \quad \frac{\Delta p}{\frac{1}{2}\rho v^2} = \left(\frac{A_{pipe}}{A_{hole}} - 1\right)^2 = 1$$

$$\frac{A_{pipe}}{A_{holes}} = 2 \quad \Rightarrow \quad \text{For } 1\,cm^2 \text{ of pipe}$$

$$A_{holes} = 0.5\,cm^2$$

→ $\delta = 1\,mm$ → To be on the safer side, take $d_{hole} = 0.9\,mm$ (say)

$$\Rightarrow A_{\substack{per\\hole}} = \pi \frac{0.9^2}{4}\,mm^2 = 0.636 \times 10^{-2}\,cm^2$$

→ For $1\,cm^2$ of pipe, $\underbrace{0.5\,cm^2}_{A_{holes}} = n_{holes} * A_{\substack{per\\hole}}$

$$\Rightarrow n_{holes} \sim 78.6 \ \frac{holes}{cm^2} \rightsquigarrow n_{holes} = 79 \ \frac{holes}{cm^2}$$

A_{pipe} ... A ... $= 1\,cm^2$ ... $= 0.012\ cm^2$ [Can use 79 and

$\rightarrow \dfrac{A_{[illegible]}}{n_{holes}} = \underset{\text{per hole}}{A_{pipe}} = \dfrac{[illegible]}{78.6 \text{ holes}} = 0.012 \dfrac{[illegible]}{\text{hole}}$ [calculate this number as well.]

$= a^2$

$\Rightarrow \underline{\underline{a = 0.112 \text{ cm}}}$ hole-centerline spacing

<u>pg.</u> 40% C_4H_{10}, 30% propane, 30% isobutane

(i)
$$X_{LFL}\Big|_{LPG} = \dfrac{1}{\dfrac{X_{C_4H_{10}}}{X_{LFL}\big|_{C_4H_{10}}} + \dfrac{X_{C_3H_8}}{X_{LFL}\big|_{C_3H_8}} + \dfrac{X_{i\text{-}C_4H_{10}}}{X_{LFL}\big|_{i\text{-}C_4H_{10}}}}$$

$$= \dfrac{1}{\dfrac{0.4}{0.018} + \dfrac{0.3}{0.022} + \dfrac{0.3}{0.018}} = \underline{\underline{0.0190}}$$

$\Downarrow$

A mixture containing 3% LPG in air is <u>flammable</u>

(ii) 0.03 mol LPG, 0.97 mol air, x mol of CO_2

$$X_{LFL}\Big|_{LPG+CO_2} = \frac{1}{\frac{X_{LPG}}{X_{LFL}|_{LPG}} + \frac{X_{CO_2}}{\cancel{X_{LFL}|_{CO_2}}_{\infty}}} = \frac{X_{LFL}|_{LPG}}{X_{LPG}}$$

$$X_{LPG} = \left(\frac{0.03}{0.03+x}\right)$$

Note: Mole fraction of LPG in the mixture of $(LPG + CO_2)$ is what matters to us in calculating LFL

(Just like $X_{C_4H_{10}}$ in "LPG" alone mattered → like 40%
• Used in (i))

$$\left[X_{LFL}\Big|_{LPG+CO_2} = \frac{0.019}{\left(\frac{0.03}{0.03+x}\right)}\right] \Longrightarrow \text{We require that}$$

$$X_{LFL}\Big|_{LPG+CO_2} > \underbrace{\left(\frac{0.03}{1+x}\right)}$$

Molefraction of LPG in the new mixture of LPG + CO_2 + air

$$\frac{0.019}{\left(\frac{0.03}{0.03+x}\right)} > \left(\frac{0.03}{1+x}\right) \Rightarrow x = \underline{\underline{0.0181}} \rightarrow \text{Moles of } CO_2 \text{ to be added}$$

X_{LPG} in mixture $= 0.02946$

In terms of mole %,

$X_{LPG} = 0.02946$, $X_{CO_2} = \frac{x}{1+x} = 0.0177$, $X_{air} = 0.9528$

Final composition

P12. Evaluate κ for (a) & (c) $\rightarrow$ Let you try (b) on your own

$$\kappa = \nabla_t \cdot \underline{u} + S_u \, \nabla \cdot \hat{n}$$

Note: $\hat{n}$ points into the fresh gases

(a) $\underline{u} = u\,\hat{e}_1 = u_1(x_2)\,\hat{e}_1 \;;\; \hat{n} = \hat{e}_2 \quad (n_1 = 0,\ n_2 = 1)$

$$\nabla_t \cdot \underline{u} = \underbrace{(1-n_1)}_{0}\frac{\partial u_1}{\partial x_1} - \cancel{\underbrace{n_1 n_2}_{0}\frac{\partial u_1}{\partial x_2}} - \cancel{\underbrace{n_2 n_1}_{0}\frac{\partial u_2}{\partial x_1}} + \cancel{\underbrace{(1-n_2^2)}_{0}\frac{\partial u_2}{\partial x_2}}$$

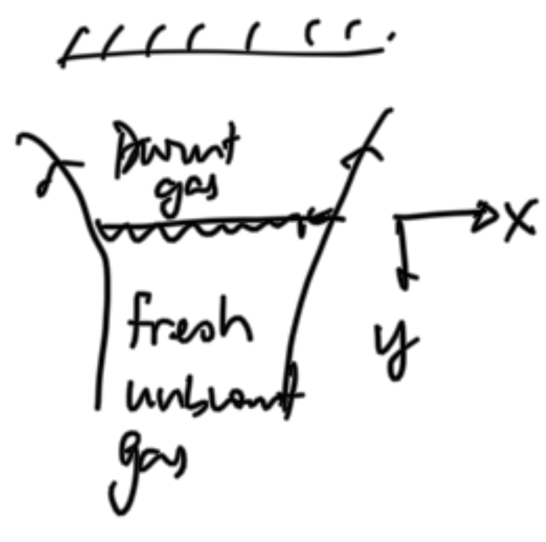
$$\nabla_t \cdot \underline{u} = \frac{\partial u_1}{\partial x_1} = 0 \quad [\text{since } u_1 = u(x_2)]$$

$$\kappa = S_u \, \nabla \cdot \hat{n} \;;\; S_u = -\underline{u} \cdot \hat{n} = u_1(x_2)\,\hat{e}_1 \cdot \hat{e}_2 = 0$$

$\Rightarrow \underline{\kappa = 0}$ $\rightarrow$ Case of an unstretched flame despite presence of flow gradients.

(c) $\underline{u} = \dfrac{ax}{k+1}\,\hat{e}_x - ay\,\hat{e}_y$

$\hat{n} = \hat{e}_y$



Final expressions:

(i) $\nabla \cdot \hat{n} = 0$

① $S_u = -\underline{u}\cdot\hat{n} = -(u_1 n_1 + u_2 n_2)$

$$S_u = ay$$

But $S_u \; \nabla\cdot\hat{n} = 0$ (OK)

② $\nabla_t \cdot \underline{u} = \dots\dots = \frac{a}{k+1}$

③ $K = \frac{a}{k+1} \Rightarrow$ constant $\rightarrow$ Case of a stretched flame, yet it is flat (planar)

Tutorial 2:

P4 Mixture fraction for real flames

$$Z_p = \sum_{k=1}^{N} a_{kp} \frac{W_p}{W_k} Y_k$$

a_{kp}: # atoms of type p in species k

Note: Z_p represents the mass fraction of the p^{th} atom at any particular location $\rightarrow$ Let us convince ourselves of this

Defn $\rightarrow Y_k = \frac{X_k W_k}{\sum X_k W_k}$ ... [illegible]

$$\sum_i X_i W_i \rightarrow \text{call this } W$$

$$\Rightarrow \frac{Y_k}{W_k} = \frac{X_k}{W}$$

$$Z_p = \sum_{k=1}^{N} a_{kp} \frac{W_p}{W_k} Y_k = \sum_{k=1}^{N} a_{kp} W_p \frac{X_k}{W} = \left(\sum_{k=1}^{N} a_{kp} X_k\right) \frac{W_p}{W}$$

$$= \left(\sum_k a_{kp} \frac{n_k}{n_{tot}}\right) \frac{W_p}{W}$$

$$= \left(\frac{n_p}{n_{tot}} \cdot \frac{W_p}{W}\right) = Y_p \quad (\star)$$

Note: The mass fraction of Y_p (like Y_C, Y_H, Y_O, Y_N) → cannot get produced or consumed — can only be transported ⇒ We should expect this quantity to be a conserved scalar. Let us prove this next.

From question: $\sum_{k=1}^{N} a_{kp} (\nu'_{kj} - \nu''_{kj}) = 0$ ⇒ This is a statement of element balance for a chemical reaction. for each element 'p'. → Call this $(\star\star)$

Conserved scalar obeys:

$$\frac{\partial}{\partial t}(\rho z) + \frac{\partial}{\partial x_i}(\rho u_i z) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial z}{\partial x_i}\right)$$

Start with species mass balance eqn:

$$\left[\sum_k a_{kp} \frac{W_p}{W_k}\right] * \left[\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k\right]$$

$$\frac{\partial}{\partial t}\Big(\rho \underbrace{\sum_k a_k \frac{W_p}{W_k} Y_k}_{=Z_p}\Big) + \frac{\partial}{\partial x_i}\Big(\rho u_i \cdot \underbrace{\sum_k a_k \frac{W_p}{W_k} Y_k}_{Z_p}\Big) = \frac{\partial}{\partial x_i}\Big(\rho D \frac{\partial}{\partial x_i}\Big(\underbrace{\sum_k a_{kp} \frac{W_p}{W_k} Y_k}_{Z_p}\Big)\Big) + \sum_k a_{kp}\frac{W_p}{W_k}\dot{\omega}_k$$

$$\Rightarrow \frac{\partial}{\partial t}(\rho Z_p) + \frac{\partial}{\partial x_i}(\rho u_i Z_p) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Z_p}{\partial x_i}\right) + \underbrace{\sum_k a_{kp} \frac{W_p}{W_k} \dot{\omega}_k}_{\star}$$

If Z_p is a conserved scalar, term $\star$ should evaluate to 0.

$\dot{\omega}_k$: Rate of prodn of the k^{th} species $(kg/m^3 s)$

Note : for a reaction j : (in general) $\sum_k \nu'_{jk} M_k \rightleftharpoons \sum_k \nu''_{jk} M_k$

Law of mass action : $\frac{1}{(\nu''_{jk} - \nu'_{jk})} \frac{d[M_k]}{dt} = \hat{\omega}_j$

Units $(1/m^3 s)$

→ Reaction rate of j^{th} reaction

(concentration)

Denotes the # of reactive collisions per unit volume per unit time

$$\dot{\omega}_{kj}\left(\frac{kg}{m^3 s}\right) = \frac{d}{dt}(\rho Y_k)\Big|_j = W_k \frac{d[M_k]}{dt}$$

Rate of production

$$\dot{\omega}_{kj} = (\nu''_{jk} - \nu'_{jk}) W_k \hat{\omega}_j$$

of k^{th} species due to the j^{th} reaction

$$\text{Total } \dot{\omega}_k = \sum_j \left(\nu_{jk}'' - \nu_{jk}'\right) W_k \hat{\omega}_j$$

Rate of production of species k over all reactions

We like to evaluate

$$\sum_k a_{kp} \frac{W_p}{W_k} \dot{\omega}_k = \sum_k a_{kp} \frac{W_p}{W_k} \sum_j \left(\nu_{jk}'' - \nu_{jk}'\right) W_k \hat{\omega}_j$$

$$= \sum_j W_p \hat{\omega}_j \sum_k \frac{a_{kp}}{\cancel{W_k}} \left(\nu_{jk}'' - \nu_{jk}'\right) \cancel{W_k}$$

$$= \sum_j W_p \hat{\omega}_j \underbrace{\sum_k a_{kp} \left(\nu_{jk}'' - \nu_{jk}'\right)}_{0}$$

$$= 0$$

from ★★ [Element Balance for any reaction j]

$\Rightarrow$ Source term vanishes!

$\Rightarrow Z_p$ is a conserved scalar

Rest of the problem is left as an exercise

P7.

$$\frac{d^2T}{dz^2} = 0$$ → to be solved on the left and right of flame with appropriate BCs.

→ Solution is obtained in terms of $T_{st} = T(z_{st})$, T_O^0, T_F^0

→ How to obtain T_{st}? → Look at the defn of z involving T say in terms of Y_F, T & evaluate at stoichiometric flame position

$$z\Big|_{st} = \frac{\left(\frac{q}{c_p} Y_F + T\right) - T_O^0}{\frac{q}{c_p} Y_F^0 + T_F^0 - T_O^0}\Bigg|_{st}$$

$$\Rightarrow \boxed{\frac{T_{st} - T_O^0}{\frac{q}{c_p} Y_F^0 + T_F^0 - T_O^0} = z_{st}}$$

Plug in numbers and evaluate T_{st} ← flame temperature for infinitely fast chemistry assumption

Final ans: (a) $T_{st} = 2237\,K$ pure CH_4/air

(b) $T_{st} = 1310\,K$ 5% CH_4 + 95% N_2 / air

P8.

(a) $T_F^0 = T_O^0 = T_0 \Rightarrow \boxed{T_{st} = T_0 + z_{st} \cdot \frac{\quad}{C_p} Y_F}$

(b) (i) $Y_F^{mix}\Big|_{st} = z Y_F^0 \Big|_{z_{st}} = z_{st} Y_F^0$

(ii) For 1 kg of fuel, let the amount of heat released be q (Heating value)

For $(z_{st} Y_F^0)$ kg fuel, the amount of heat released $= q z_{st} Y_F^0$

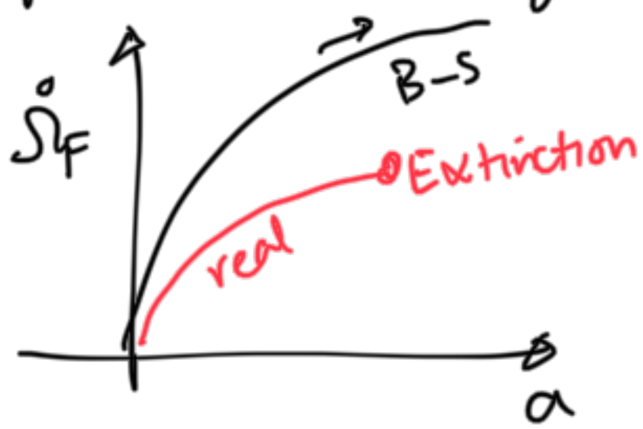
$$C_p \left(T_{prem}^{ad} - T_0\right) = q Y_F^0 z_{st}$$

$$\boxed{T_{prem}^{ad} = T_0 + \frac{q}{C_p} Y_F^0 z_{st}}$$

Same

P10. Discussed in Thierry Poinsot, section §3.4

Finally, after all math, you will see that $\dot{S}_F \propto \sqrt{a}$ for Burke-Schuman solution → not realistic since there is no point of extinction



The true scenario is as shown in red