AE4262–Combustion for Propulsion and Power Technologies

Oral Exam Notes

Handwritten Notes on the Series of 14 Lectures Given by I.Langella, F. de Domenico, and G. Kelesidis

April-June 2025

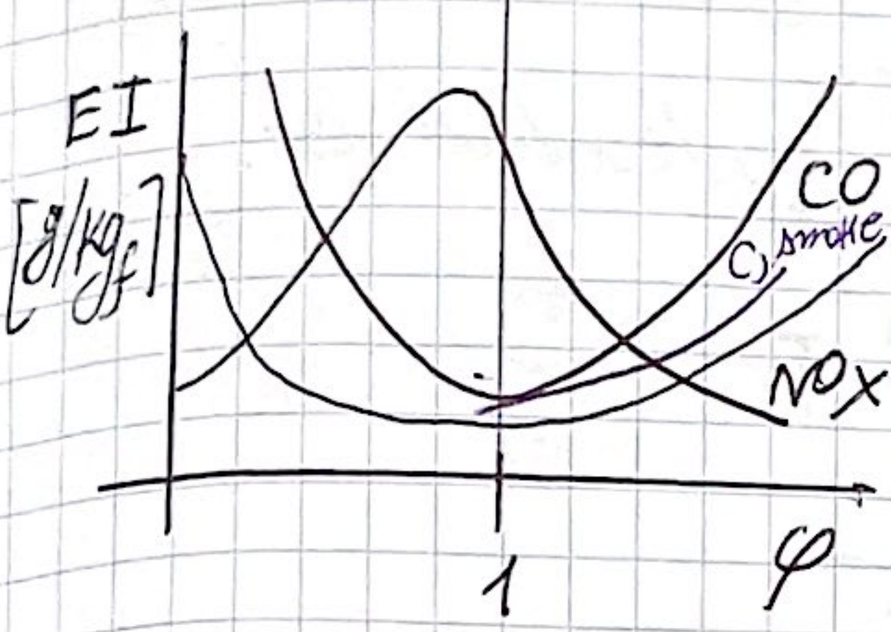
Jakub Bartmański

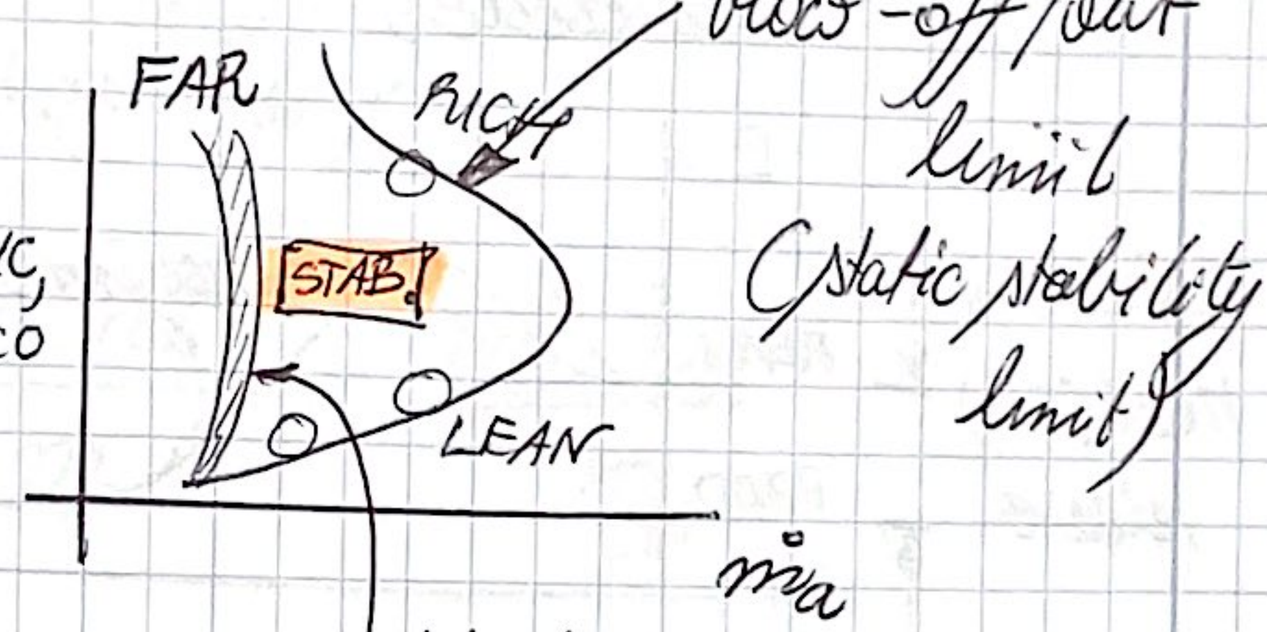
COMBUSTION - EXAM NOTES

(1) 1. Emissions not only are about CO_2 — some species produced prevalently @ high T or rich $\varphi > 1$, some — the opposite

Real concentrations may be diff than equilibrium concentrations due to short residence times

UHC & Soot also important





○ ≡ HF oscillations

2. Reacting gas is a non-isothermal mixture, where species must be tracked enclividually and each heat coeffs vary ∝ T.

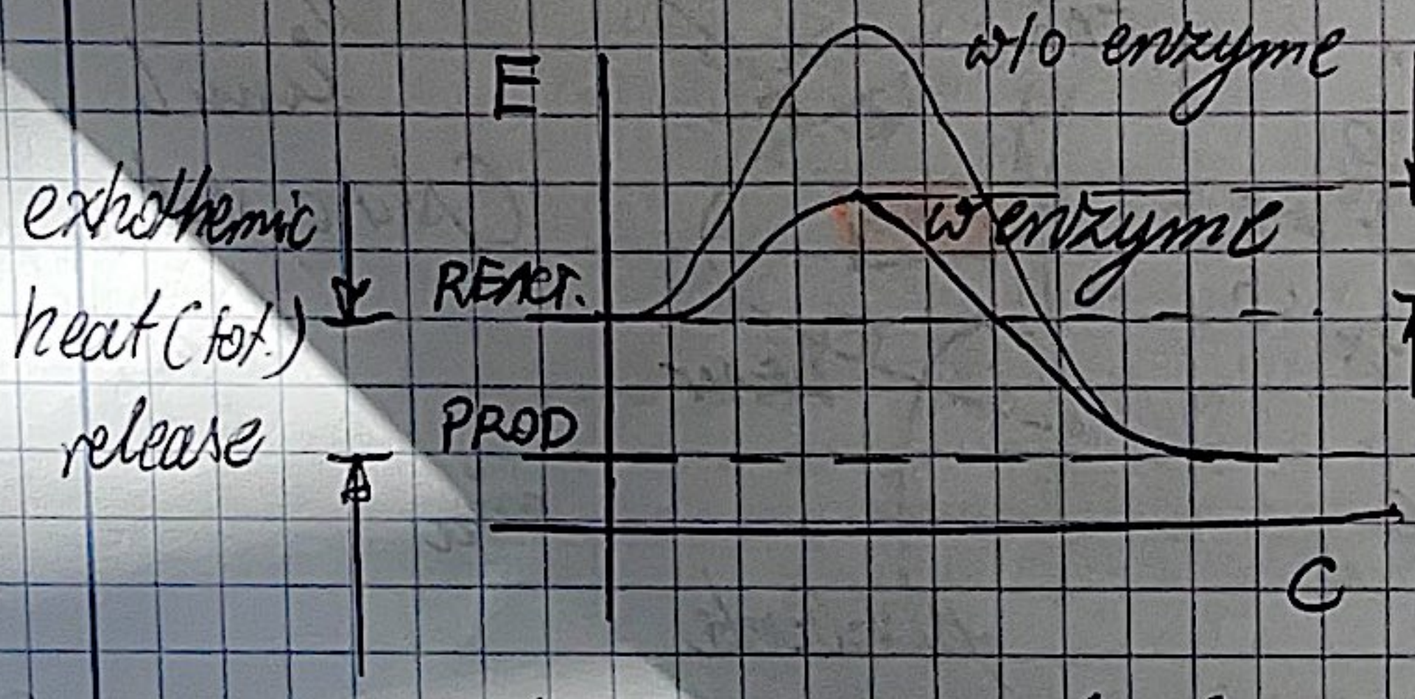
3. Everything is Coupled: Reaction rate (T), T (Rea. rate), c_p (T), c_p (p) ... (2)

- Transport coefss (species, T)
- As T varies as a result of heat release, TDs, flow & transport variables are strongly cpld.

4. Combustion characterized by:

- oxidation (reducing agent $^{2-}$ loses $2xe^- \rightarrow Ox$
- exothermic
- high activation energy, high T & self sustaining

although @ first gotta provide en to brake the bonds of the molecules



5. Most common fuels are organic — Hydrocarbons (other fuels possible, ex: F, Al, B ...)

6. • Usually $\eta_{cc} > 99\%$, but that 1% of inefficiency is related/responsible, too, for toxic emissions (CO & NOx)

$EMI \sim \frac{1}{\eta_{cc}}$ → $\eta_{cc}\uparrow$ then less toxic emissions!

• Sometimes, tho, some pollutants like soot are desirable — soot is an aerosol which reflects incoming radiation: $RF < 0$ (?)

7. Combustion variables

$\rho, u_i, S, T, h, Y_K, 1 \leq K \leq N, N > 50!$

$$Y_K := \frac{\text{mass of species (s) } K}{\text{total mass}} \quad \text{mass fraction}$$

$$X_K = \frac{\#\text{ of moles of } S_K}{\#_{tot.}\text{ moles}} \quad \text{mole fraction}$$

$$[X_K] = \frac{\#\text{ of moles of } S_K}{\text{volume, tot}} \quad \text{molar concentration}$$

W_K = molar mass $\left[\frac{g}{mol}\right]$

note

$$Y_K = \frac{m_K}{m} = \frac{W_K n_K}{m} = \frac{W_K X_K}{\frac{m}{n}}$$

and $\frac{Y_K}{W_K} = \frac{\cancel{m_K}}{m} \frac{n_K}{\cancel{m_K}} = \frac{n_K}{m}$, so

$$\sum \frac{Y_K}{W_K} = \frac{\sum n_K}{m} = \frac{n}{m}, \text{ so}$$

$$Y_K = W_K X_K \sum \frac{Y_K}{W_K}, \text{ or}$$

$$X_K = \frac{W}{W_K} Y_K, \text{ with } W \equiv \left(\sum_K Y_K / W_K\right)^{-1}$$

also

$$[X_K] = \frac{n_K}{\vartheta} = S \frac{n_K}{m} = S \left(\frac{n_K}{m_K}\right)\left(\frac{m_K}{m}\right)^{1/W_K} Y_K$$

$$[X_K] = S\, Y_K / W_K, \quad S \text{ of cell mixture.}$$

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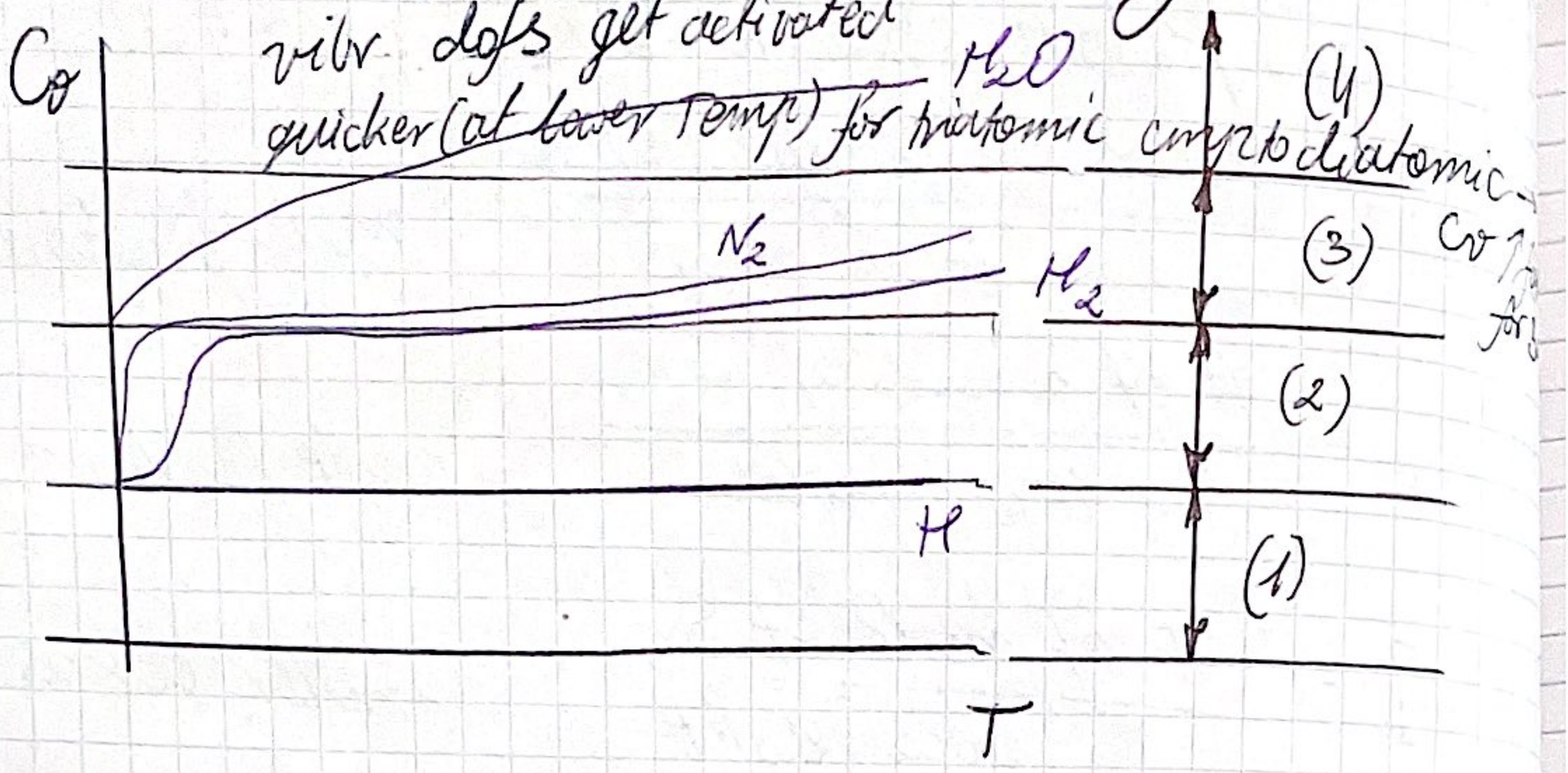
note

Knudsen #

$S(x,t)$ is B.V. So assume continuum — assumed smaller than any phys. structure (like small vortex), but still > than size of molec.

the smallest el in domain is

8. Dxiation of molar heat capacity



(i) ≡ contribution of :

- (1) transl.
- (2) rot.
- (3) vibr.
- (4) vibr.

EXCITATION

—

of diatomics
of diatomics.
of polyatomics

If $T\uparrow$, then KE ↑, but only up to some pt. @ some T, some of the thermal energy is used to excite rot, transl & vibr DOFS, thereby increasing C_v, C_p. (DOF of a molecule can ↑ due to $T\uparrow$, so also C_p, C_v) → that's why $C_p \neq$ const.

" @ ambient T the most stable particle config is a diatomic molecule "

IL

9). For a species K, the (total) enthalpy is :

- $h_K = \underbrace{\int_{T_0}^{T} C_{p,K}\,dT'}_{\text{sensible}} + \underbrace{\Delta h^\circ_{f,K}}_{\text{chemical}}$

$T\uparrow \Rightarrow H_1 \rightarrow H_2$ (Assume H_1 is stable molecule)
dof H_2 > dof H_1, so δq is "absorbed" by H_2 (more dofs- but not Temp rise)
$(T+\delta_q)$
T
δq
$S = \frac{S}{\text{unit mole}}$

and $T_0 := 298,15\ [K]$ ($T_0 = 0\ [K]$ would be impractical)

- So basically entalpy is defined exactly as a copy, but sensible enth. is 0 @ $T = T_0$, and then $h_k = \Delta h^\circ_{f,k}$.
- $\Delta h^\circ_{f,k} \equiv$ the MASS (per unit kg) enth of formation of species k @ T_0
- Can also define molar enthalpy of formation

$$\Delta h^{\circ,m}_{f,k} := \Delta h^\circ_{f,k} \cdot W_k .$$

10. Defs.

$C_v = C_v\ min$

@ $v = const$ $\quad dU = \delta Q = C_v\, dT$

@ $p = const$ $\quad dH = \delta Q = C_p\, dT$

@ $v = const$ $\quad U(T) = U^\circ + \int_{T_0}^{T} C_v\, dT$

@ $p = const$ $\quad H(T) = H^\circ + \int_{T_0}^{T} C_p\, dT$

if reversible: $T\,dS = \delta Q$, so

@ $v = const$ $\quad dS = C_v \frac{dT}{T}$, so

$$S(T) = S^\circ + \int_{T_0}^{T} \frac{C_v}{T}\, dT$$

@ $p = const$:

$$S(T) = S^\circ + \int_{T_0}^{T} \frac{C_p}{T}\, dT$$

See that for rev $dS = c\frac{dT}{T}$, so entropy (rev) is a state → for rev, S doesn't depend on path (makes sense)

H.

ΔH_f° → @ T_0 & $p = 1$ bar

f → formation

→ enth. of formation

→ "difference from a state that we can compr it to "1L"

→ Relative change from starting biatomic species to the products. The enthalpy of biatomic is by def 0.

$\Delta H_f^\circ > 0$ → energy must be added to form the species.

$\Delta H_f^\circ < 0$ → energy is released during formation of species starting from biatomic.

"It is not possible to quantify the absolute enthalpy and enthalpy energy of a compound, but relative changes in these quantities can be estimated — it's given by a weighted sum":

$$h := \sum_K h_K Y_K \quad \left(\text{or } h \doteq \sum_K h_K^m X_K\right)$$

Then $h = \sum_k Y_k h_k = \sum_k Y_k \left(\Delta h_{f,k}^\circ + \int_{T_0}^{T} C_{p,k}\, dT' \right)$

$= \int_{T_0}^{T} \left(\sum_k Y_k C_{p,k} \right) dT' + \sum_k \Delta h_{f,k}^\circ Y_k$

$= \int_{T_0}^{T} C_{p,mix}\, dT' + \sum_k Y_k \Delta h_{f,k}^\circ$

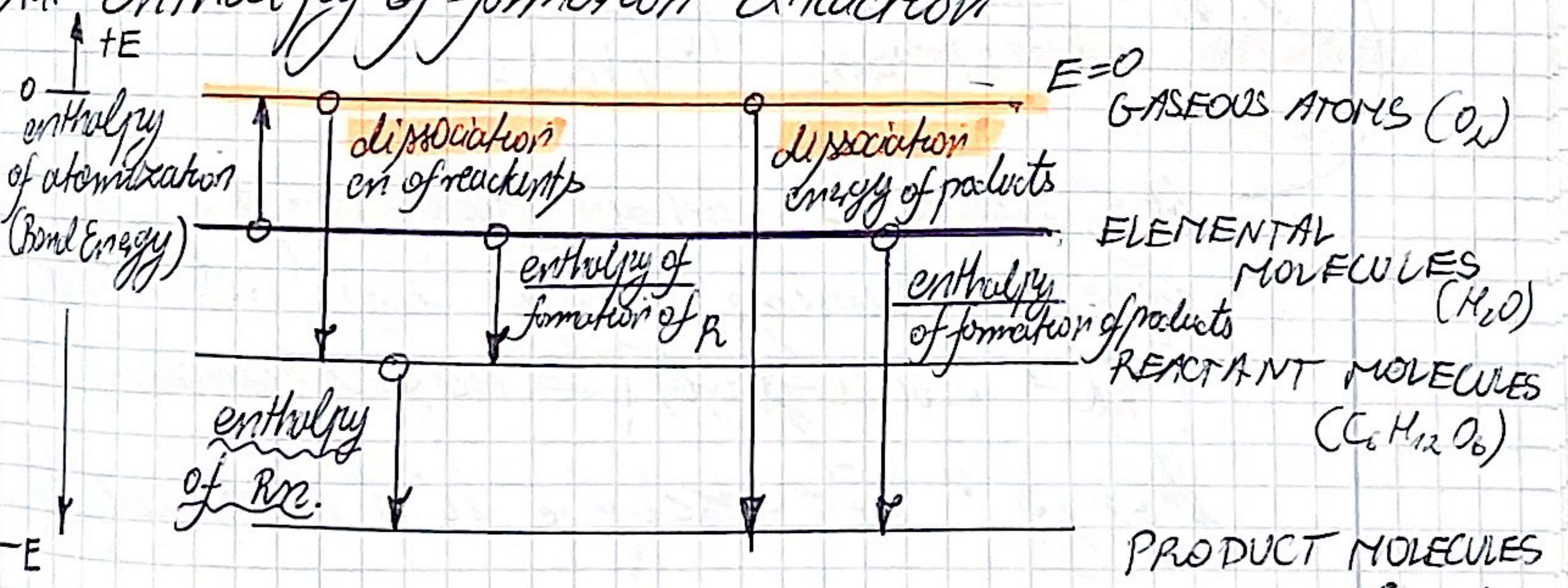
by def $C_{p,mix} := \sum_k Y_k C_{p,k}$.

and similarly u_{mix}, S_{mix}, ...

12 Hess law: "If a rn (usb or usch.) is carried out in stages, the algebraic sum of the heat evolved in separate stages is = to the total amount of heat released when the rn ours directly". " It means that heat liberated in a reaction is indep of the path of the rn betw the init & final states".

13. "Gaseous atoms are less stable"

14. Enthalpy of formation & reaction



15. "Energy which can be Tf in a cc pcess is obtained by breaking the bonds which hold the fuel atoms together"

16. Revisit L1, s. 37 → think what has bigger what & (e.g.), why alcohols are not used so much in engines (AeroEngn)

17. Some observations (on the table above)

- ΔH_R of many hydrocarbon fuels on mass basis is similar $\approx$ 40-50 MJ/kg
- $FAR_{st} \in [1/17 ; 1/13]$ + almost hydrocarb.
- some fuels have ⊕ve enth of formation
- ALL —"— ⊖ve reaction!
- common fuels ∃ a mix of several hydrocarbons
- ΔH_R per kg for alcohols is < (<) than non-oxygenated fuels (as oxygen doesn't provide energy of reaction).

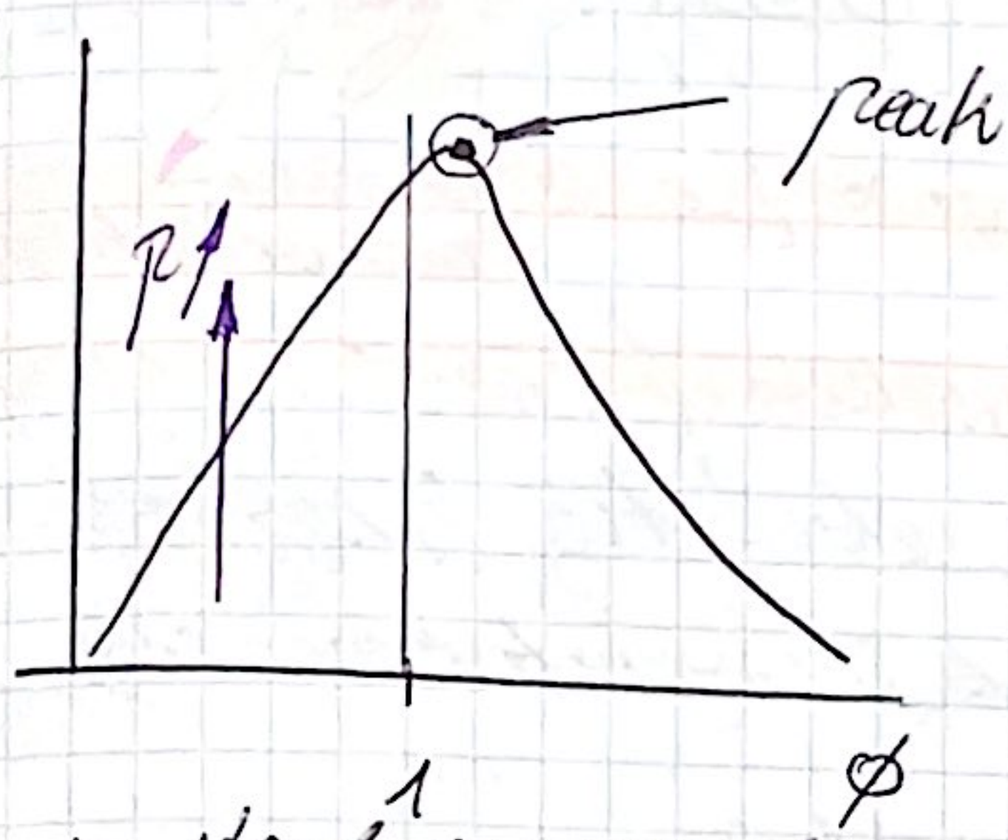
18. Use LHV not HHV cuz ya can't store condens. energy en aero-eng

(2) 1. T_{ad} → temp of P when $\delta Q = 0$: $h_p(T_{ad}) - h_r = 0$

2. $\phi = \dfrac{\dot{m}_f / \dot{m}_{ox}}{(\dot{m}_f / \dot{m}_{ox})_{st}} = \dfrac{Y_F / Y_{ox}}{(Y_F / Y_{ox})_{st}}$

→ Also, due to 1L: Adiab flame temp: you're assuming a 0D lumped model [$T_{bl} \neq T_{ad}(x\text{-grid})$] — no gradients, homog." We assume also complete c

3.



Why peak not @ $\varphi = 1$?

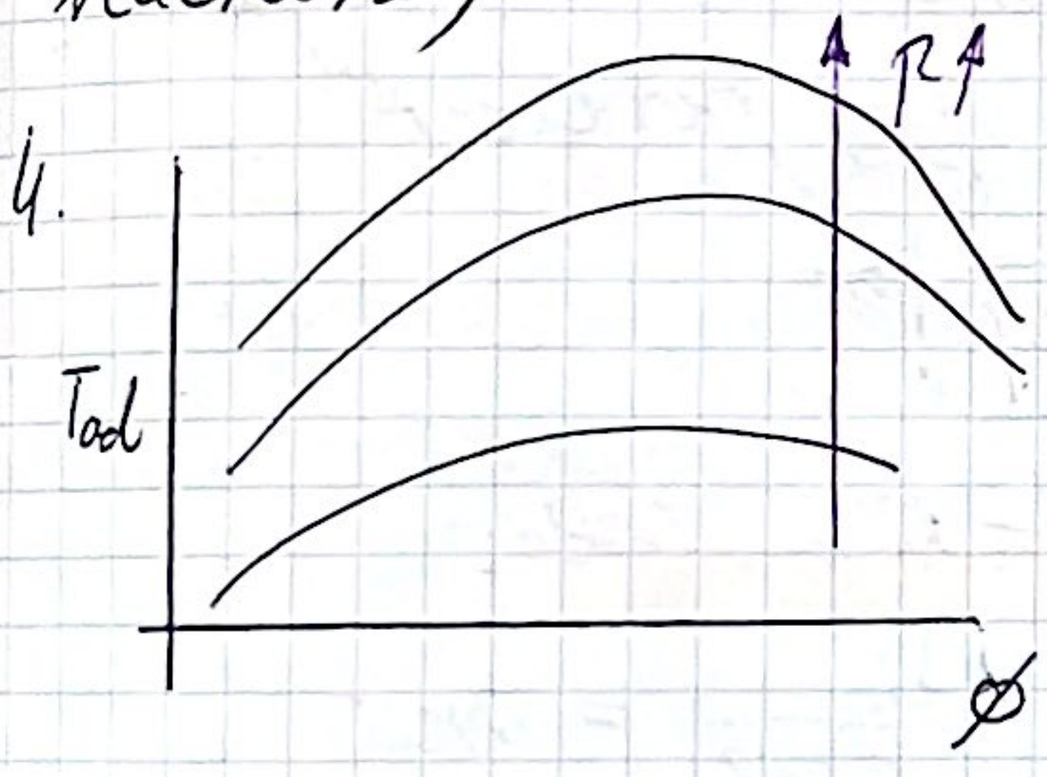
1) @ $\varphi = 1$, max heat release, not T_{ad}

2) @ $\varphi > 1$ ∃ shortage of oxygen so less dissociation reactions which are endothermic, so steal energy (energy goes into bond breaking, instead of increase in T_{ad})

3) In $\varphi > 1$ the products include not fully oxidized species (CO, H_2), whose C_p is less compared to fully oxidized counterparts (CO_2, H_2O)

4) @ $\varphi = 1$ products more fully oxidized, but the energy release is partitioned, amongst others, into vibrational excitation of molecules. (+ endoth. reactions)

4.



Why T_{ad}↑ with p↑?

1) Dissociation reactions which are endothermic:

$$H_2O \underset{\text{formation } \Delta H<0}{\overset{\text{diss. } \Delta H>0}{\rightleftharpoons}} \frac{1}{2}O_2 + H_2$$

&

$$CO_2 \rightleftharpoons CO + \frac{1}{2}O_2$$

are suppressed. Furthermore, due to the Le Chatelier's Principle, the equilibrium will toward fewer moles of gas (left side) — this suppresses dissociation.

2) @ high p the rxn rates are enhanced which makes the combustion complete & release more

energy per mole - chatty (?)

5. Tad with: causes $\gamma_{cc} = 1$ & cannot predict minor species.

Hp: complete combustion (ever?), 1 step, ∞-fast chemistry, adiabatic & isobaric process; OD (no transport & convective processes)

$$F + O_2 \rightarrow CO_2 + H_2O$$

also: complete implies ever & 1-step

conservation of mass says:

$$(1) \quad \frac{\Delta n_k}{\Delta \nu_k} = \xi = \text{const} \quad \forall_k$$

with the convention that $\nu_k^{PROD} > 0$

$\nu_k^{REACT} < 0$

"species get consumed & produced @ the same rate: 1 mole of fuel consumed is 1 mole (per ν) produced of a(ny) product"

For 1-step chemistry

divide (1) by $n = \frac{1}{\bar{\nu}} n_i$, then

$$\frac{\Delta X_k}{\Delta \nu_k} = \text{const}, \text{ or } \frac{\Delta Y_k}{W_k \Delta \nu_k} = \text{const}$$

Now,

$$h^{PROD}(T_{ad}) - h^{REACT}(T_R) = 0$$

$$\sum Y_{i,R} \Delta h_{f,i}^{0} + \int_{T_0}^{T_R} c_{p,r} dT' = \text{---} \text{"} \text{---}$$

so $\underbrace{\sum(Y_{i,r} - Y_{i,p})\Delta h^{\circ}_{f,i}}_{A} = \int_{T_0}^{T_p} C_{p,p}\,dT' - \underbrace{\int_{T_0}^{T_r} C_{p,r}\,dT'}_{\approx 0,\ as\ T_r \approx T_0}$

now

since $\frac{\Delta Y_F}{W_F \nu_F} = \frac{\Delta Y_K}{W_K \nu_K} \Rightarrow \Delta Y_K = \frac{\Delta Y_F}{\nu_F W_F} \cdot W_K \nu_K$

so $A = \frac{\Delta Y_F}{\nu_F W_F} \underbrace{\sum_K W_K \nu_K \Delta h^{\circ}_{f,K}}_{\Delta H_R =}$ ← heat of RN

$= \int_{T_0}^{T_p} C_{p,p}\,dT'$ & RHS $\equiv \langle C_{p,p} \rangle (T_p - T_0)$

So $T_p = T_0 + \frac{\Delta H_R Y_{F_r}}{\langle C_{p,p} \rangle \nu_F W_F} + \frac{\langle C_{p,r} \rangle}{\langle C_{p,p} \rangle}(T_r - T_0)$ if $\phi \le 1$

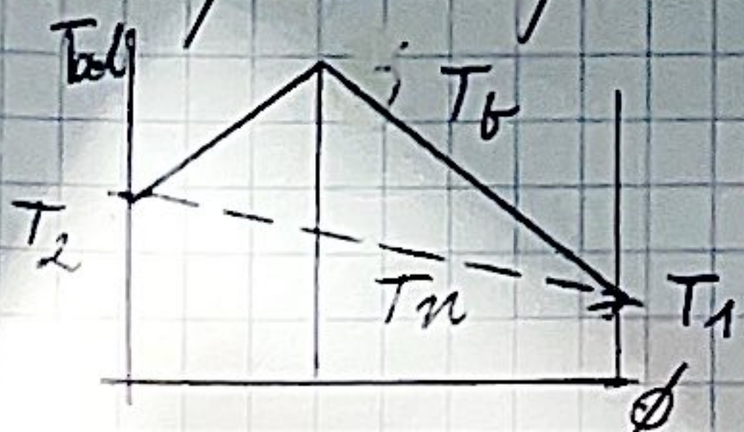
&

$T_p = T_0 + \frac{\Delta H_R Y_{ox,r}}{\langle C_{p,p} \rangle \nu_{ox} W_{ox}}$ + —11— if $\phi > 1$

$\Delta Y_i = Y_{i,r} - Y_{i,p}$ & if $\phi > 1 \Rightarrow Y_{ox,p} = 0$
else $Y_{F,p} = 0$, that's why you see this case breakdown.

- Note $\langle C_p \rangle_{reac} < \langle C_p \rangle_{pod}$. (due to massive ΔTemp)
- Heat-balance-Tool is the ultimate upper bound on Tad!

- Overpredicts peak!



$T_b \uparrow$ if $\phi \uparrow < 1$ as then $Y_F \uparrow$
$T_b \downarrow$ if $\phi \uparrow > 1$ $Y_{ox} \downarrow$

6. Some notes from L1&2 notes: but only for single species

- assume ideal gas law + considerations. Works well $\leq 5K$ [K]: $p_K = \frac{n_K}{V_K} R_0 T$

use dalton:

$$p = \frac{\sum_K}{K} p_K$$

Because: $V_K = \frac{m_K}{n_K}$;

$$p_K = \frac{n_K}{V_K} R_0 T = \left(\frac{m_K}{V_K}\right)\left(\frac{R_0}{W_K}\right) T = \frac{g_K}{K} R_K T$$

$g_K = R_K$

$$\text{So } p = \frac{\sum_K}{K} g_K \frac{R_0}{W_K} T = R_0 T \frac{\sum_K}{W_K} \frac{g_K}{W_K} =$$

$$= g R_0 T \frac{\sum_K}{W_K} \frac{V_K}{W_K} = g \frac{R_0}{W} T$$

- entropy = measure of disorder or # of microstates for a fixed macrostate
- Clausius says: $\oint \frac{\delta Q^{Rev}}{T} = 0$ even though $\oint \delta Q \neq 0$, since Q is not a state! So $\delta Q^{rev}/T$ is a state! Further

$$\int_1^2 \frac{\delta Q^R}{T} = S_2 - S_1$$ (if I didn't have Clausius, I wouldn't have known that $\delta Q^R/T$ is state, so the symbol LHS could have an arbitrary value assigned depending on path!

Differentiating: $\delta Q^{Rev} = T dS$. (max vars)

• can show $Dq = dh = du + pdv + vdp$
if isobaric, then $vdp = 0$. Then this eqn tells you that in an isobaric process the heat is totally used to produce work which can be exploited (in isochoric not). Is there a proces nearly isobaric? Yes! Deflagration (flame condition en motfcc - ~~Otto, Diesel~~ detonation is isochoric! So doesn't yield useful work produced during cc! Despite that, it don't mean you can't extract work in a detonation proces. It just means work is not produced as you cc. (@cost of lower η).

• PRZECZYTAJ ŻÓŁTE NOTKI w lecture notes

• Nauc na pamięć równania rms if $\phi \in (0, \infty)$. Which is basically the fact that you have

$$(n \cdot F, n_{ox}) = \begin{cases} (1, \phi), & \phi < 1 \\ (\phi, 1), & \phi \geq 1 \end{cases}$$

So:

$$\phi F + \nu_{O_2}\,(O_2 + 3{,}76 N_2) \xrightarrow{\phi} \nu_{CO_2} CO_2 + \nu_{H_2O} H_2O + 3{,}76\,\nu_{O_2} N_2 + \nu_{O_2}(1-\phi) O_2 \quad \text{for } \phi < 0$$

Współ. ν is the "balance" coeff IF @ Stoich. n is the same but if not

AND

$$\phi F + (O_2 + 3{,}76 N_2) \longrightarrow \nu_{CO_2} CO_2 + \nu_{H_2O} H_2O + 3{,}76\,\nu_{O_2} N_{2\,@\,\text{stoich.}} + \nu_f (\phi - 1) F$$

ν → stoich coeffs.
n → real/non-stoich.

can show: $\phi = \frac{\nu_{ox}}{\nu_F} \frac{(nF)}{(n_{ox})}$ ← to get coeffs

Współ. ν to coeff, który nie zmienia się w reakcji → # of moles does not change in the reaction

- Categorize cc process en :

— autoignition & explosion :
perfect & stirred reactor where
gas mixture is homog & any stage, so
$\nabla \equiv 0$. So no diff or conv effs.
Explosion = condtn for which a
sufficient # of radicals is present in
the mixture so that a reaction then
is triggered characterized by a exp
growth of Radicals. This can be
achieved by assisted ignition (spark) or
for certain operative conditions, is preceded
by autoignition — where R are produced
@ slower rates then en explosion,
until expl. is reached.

— Propagation : Combustion pops
differ here @ (x, t) allowing for
diffusion & conv processes — or,
more generally — transport poceses.
This allows for defn of a flame :=
:= "hot glowing body of ignited gas".
We will talk ab flame font ? — so
flame with a LE propagating thru
the reactant mixture.

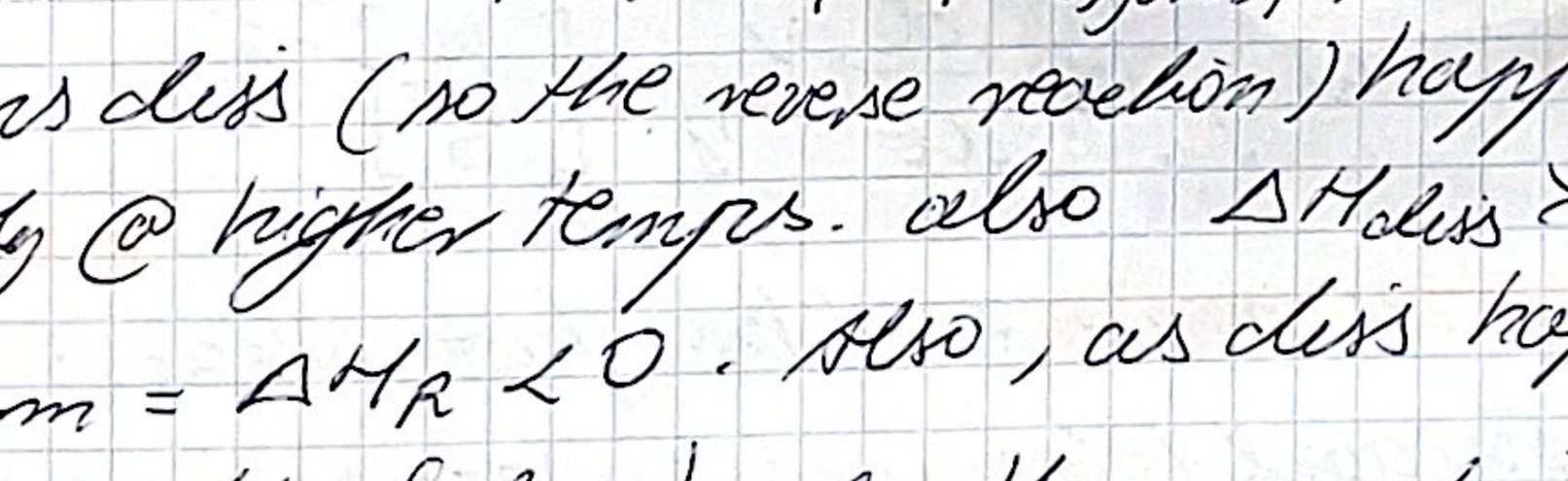
7. ~~Equilibrium~~ Kinetic chemistry — Tool

Assume: reversible chemistry, account for dissociations, can predict minor species, assume diss — II — ave @ equil., cc not complete yo $\gamma \neq 1$ (but maximum possible — upper limit), assume ∞-fast chemistry so will not take into account time scales, 0D (no transport processes)

E.g. Dissociation rx:

$$CO_2 \rightarrow CO + \tfrac{1}{2} O_2 \quad (-\text{energy})$$

so $\Delta H > 0$. See:



formation, exothermic, (cc)

dissociation, endoth

So observe now $|Ea, diss| > |Ea, form|$, which means diss (so the reverse reaction) happens mostly @ higher temps. also $\Delta H_{diss} > 0$, while $\Delta H_{form} = \Delta H_R < 0$. Also, as diss happens, it yo Probability of less ↓. So there must ∃ a balance where fwd & reverse reactions balance.

Consider now a homog, adiabatic system and a jth reversible reaction with stoich coeffs ν:

$$\nu_A' A + \nu_B' B \rightleftharpoons \nu_C'' C + \nu_D'' D$$

define $\nu := \nu'' - \nu'$

mass:

$$\nu_A' W_A + \nu_B' W_B = \nu_C'' W_C + \nu_D'' W_D$$

$$\sum_i^{N_R} \nu_{j,i}' W_i = \sum_o^{N_P} \nu_{j,o}'' W_o \quad \text{or}$$

Or taking a whole set of indices $k \in K$

$$K = A \cup B$$

$$\sum_k^{N_R \cup N_P} \nu_{j,k}' W_k - \nu_{j,k}'' W_k$$

$$\boxed{\text{or} \quad \sum_k^{N_R \cup N_P} \nu_{j,k} W_k = 0}$$

Now, define a REAN-RATE of species k in rxn j:

$$\dot{\omega}_{k,j} := \frac{d}{dt} Y_{k,j} \left[\frac{kg}{s}\right]$$

$\dot{\omega}$ is a measure of how fast species k is produced / destroyed in rxn j.

For most temps (as rxn starts), reactants are destroyed @ rate faster than produced

in the reverse rn (deto lower E_a) as $T \uparrow$, the production of reactans increases, until some T_0 where the rates are the same → chemical equilibrium → this is the essence of chem. eq. method.

The sum of consumptions of species K in all M reactions:

$$\dot{\omega}_K = \sum_j^M \dot{\omega}_{K,j} \text{), and also } \sum_K \dot{\omega}_K = 0$$

remember how $\frac{\Delta n_K}{\Delta \nu_K} = \xi = \text{const} \; \forall_K$? (can prove from $\sum \nu_{jk} W_k = 0$ & def of $\dot{\omega}_{Kj}$)

It means rxns, no rate of production/destruction is in stoichiometric proportions. ξ is the extent of rn.

This somehow implies $\frac{\Delta Y_K}{W_K \nu_{K,j}} = \text{const} \; \forall_K$

dividing by $\Delta t \to 0$:

$$\mathcal{Q}_{K,j} = \text{const} \; \forall_K = \frac{\dot{\omega}_{K,j}}{W_K \nu_{K,j}} = \mathcal{Q}_j, \text{ indep of } k$$

$\mathcal{Q}_j$ = rate of progress of reaction j. At eq, $\mathcal{Q}_j = 0$, so fwd & reverse rns rates must be the same. This is a dynamic eq! Species still being converted back & forth but only @ the same rate.

But $\mathcal{Q}_j = K_{fj} \prod_K [X_K]^{\nu'_{kj}} - K_{rj} \prod_K [X_K]^{\nu''_{kj}} =$

$= f(T, p, Ea, \ldots)$ ⟶ need to access chemistry for that! Is there an easier way?
Yes ⟶ TD., We need a criterium of spontanity. (When are f & r equal?)

Utilize II TD: $\Delta S_{universe} = \Delta S_{system} + \Delta S_{surroundings} \geq 0$

"Gibbs realized that for a reaction, a certain amount of energy goes into an increase in entropy of a system and a certain amount goes to a heat exchange for a rxn":

Define Gibbs energy $G = H - TS$
G is state, too. This way, the differential dG does not depend on path, so might as well choose any process. choose isothermal for convenience:

$dG = dH - TdS + SdT \neq 0$

Now assume:

- reversible process: $\delta Q = TdS$
- closed system (no mass exch w surroundings)
- Isobaric process $\delta Q = dH$

(← above: isoTh.)

II TD: $dS_u = dS_{sys} + dS_{surr}$

Use assum of rev : $dS_{surr} = \frac{\delta Q_{surr}}{T}$

but $\delta Q = \delta Q_{surr} + \delta Q_{sys} = 0$, so

$$dS_u = dS_{sys} - \frac{\delta Q_{sys}}{T} = dS_{sys} - \frac{dH_{sys}}{T}$$

if system @ eq then $dS_u = 0$, otherwise $dS_u > 0$, so

@ equil : $dG_{sys} = dH_{sys} - TdS_{sys} = 0$

not @ equil : $dG_{sys} =$ " < 0

So if sys not @ equil, then $dG < 0$ represents the "excess energy" liberated @ non eq. cdtns. Part of heat goes into an increase of entropy (or temp), but @ non-eq, part of the heat is used for reaction progress (free energy). If process isoth, not isob, then use Helmholtz free energy : $F = U - TS$. Note

$G - F = H - U = PV > 0 \Rightarrow G > F$.

So free energy is larger for an isobaric process.

When $\Delta G > 0$ → procs is endergonic = not spontaneous in fwd direction. It's spontaneous in reverse direction to make more starting material

When $\Delta G < 0$ → exergonic → spont. form more products

$\Delta G = 0 \rightarrow$ dynamic equil, concentrations are constant of time

- if $\Delta H < 0$ & $\Delta S > 0 \Rightarrow \Delta G < 0$, so reaction always spont. Usually combustion: $\Delta H_R < 0$ & more product molecules so $\Delta S > 0$.
- $\Delta H < 0$ & $\Delta S < 0$. If Temp low enough, $\Delta G < 0 \rightarrow$ condensation: exothermic but $\Delta S < 0$ @ const temp cuz DOF ↓ (liquid to solid)
- $\Delta H > 0$ & $\Delta S > 0 \rightarrow \Delta G < 0$ provided Temp is large. Thus is the case for dissociation reactions. ($\Delta S > 0$ ↑ due to more molecules, endothermic). Enough high temp is equiv to having enough high Ea.
- $\Delta H > 0$ & $\Delta S < 0 \Rightarrow \Delta G > 0$, never spont. It doesn't mean it doesn't occur in nature, but just we need to provide energy to happen. Photosynth. eqn's.

Start: dG and choose with:

$dG = dH - TdS$

but if sys rev: $dU = TdS - pdV$

So

$dH = \overbrace{dU + pdV}^{TdS} + Vdp = TdS + Vdp$

ΔS bcs more molecules to be understood as eg glucose (more molecules), not nec. Temp, Temp ↑ more microstates

So $\underline{dG} = TdS + Vdp - TdS = \underline{Vdp}$

for a single species K & ideal gas enthalpy:

Gibbs per mole:

$$G - G^\circ = \int_{p_0}^{p_K} \frac{R_0 T}{p'} dp' = R_0 T \ln \frac{p_K}{p_0}$$

(g)

$$G_K - G_K^\circ = R_0 T \ln\left(\frac{p_K}{p_0}\right)$$

So $G_P = \sum_{a \in P} n_a G_a$, $G_{Reactants} = \sum_{b \in R} n_b G_b$

So

$$\Delta G_{REACTION} = G_P - G_{Reactants} = \sum_i n_i G_i$$

$$= \underbrace{\sum_i n_i G_K^\circ}_{0} + \sum_i R_0 T \ln\left(\frac{p_i}{p_0}\right)^{n_i}$$

$\Delta G_{REACTION(R)} \equiv$ standard Gibbs energy i.e. @ 1bar

and since $\Delta n_i = \xi \Delta \nu_i$ or simply

$= \xi \nu_i$ $(\nu_i = \nu_i'' - \nu_i')$,

then:

$$\Delta G_R = \Delta G_R^\circ + \sum_i RT \ln\left(\frac{p_i}{p_0}\right)^{\nu_i}$$

(+ve when ν_i'', +ve when ν_i')

$$= \Delta G_R^\circ + RT \ln \prod_i \left(\frac{p_i}{p_0}\right)^{\nu_i}$$

@ equilibrium $\Delta G_R^{\,i} = 0$, so

$$\underbrace{\prod_i \left(\frac{p_i}{p_0}\right)^{\nu_i}}_{\text{reaction quotient}} = \exp\left\{-G_R^\circ(T)/RT\right\} =: \underbrace{K_p(T)}_{\text{eqil. constant.}}$$

if $K_p(T)$ the equil constant is $> 10^3$, then the reaction is strongly shifted twd products & combustion is almost complete. if $< 10^{-3}$ then shifted twd reactants so the reverse rxn is almost complete.

note $p_i = X_i p$ (Dalton)

Consider

$$\nu_A' A + \nu_B' B \rightleftharpoons \nu_C'' C + \nu_D'' D, \text{ then}$$

$$\left(\frac{p}{p_0}\right)^{[(\nu_C''+\nu_D'')-(\nu_A'+\nu_B')]} \frac{X_C^{\nu_C''} X_D^{\nu_D''}}{X_A^{\nu_A'} X_B^{\nu_B'}} = K_p(T) = e^{-\frac{\Delta G_R^\circ}{R_0 T}}$$

$p_0 = 1 \text{ bar}$

Consequences:

- T↑ : exponent RHS $\sim \frac{1}{T}$. If cc & ~~exo~~thermic ($\Delta H_R^\circ < 0$), then $\Delta G_R^\circ > 0$ (cuz entropy increases, cc), so $e^{+\downarrow}$ means RHS↓ $\Rightarrow K_p \downarrow$. So, @ p = const, mole fractions of products have to ↓ or reactants ↑, so reaction moves twd reactants. In other words, the response to T↑ is that the system favors reverse reactions (endothermic in this case), which

would steal energy to decrease overall temp! → Le Chatelier → system reacts opposite to external prompt (reactor prekony) → form of conservation of energy (↑ T↑ ⇒ T↑ then exponential growth out of nowhere. Must have T↑ ⇒ T↓)

- Change of concentrations. For P, T const if increase reactants or subtract products, the system has to do the opposite to keep $k_p(T = \text{const}) = \text{const}$. So increasing reactants has to mean increase products, so equil shifts towd products (Chatelier)
- Change of pressure if T = const, then if:

a) $\sum \nu = 0$, e.g.

METHANE CC $CH_4 + 2O_2 \rightleftharpoons 2CO_2 + H_2O$, then
(3) (3)

pressure has no effect

H_2 CC b) $\sum \nu < 0$, e.g.

$$2H_2 + O_2 \rightleftharpoons 2H_2O$$
(3) (2)

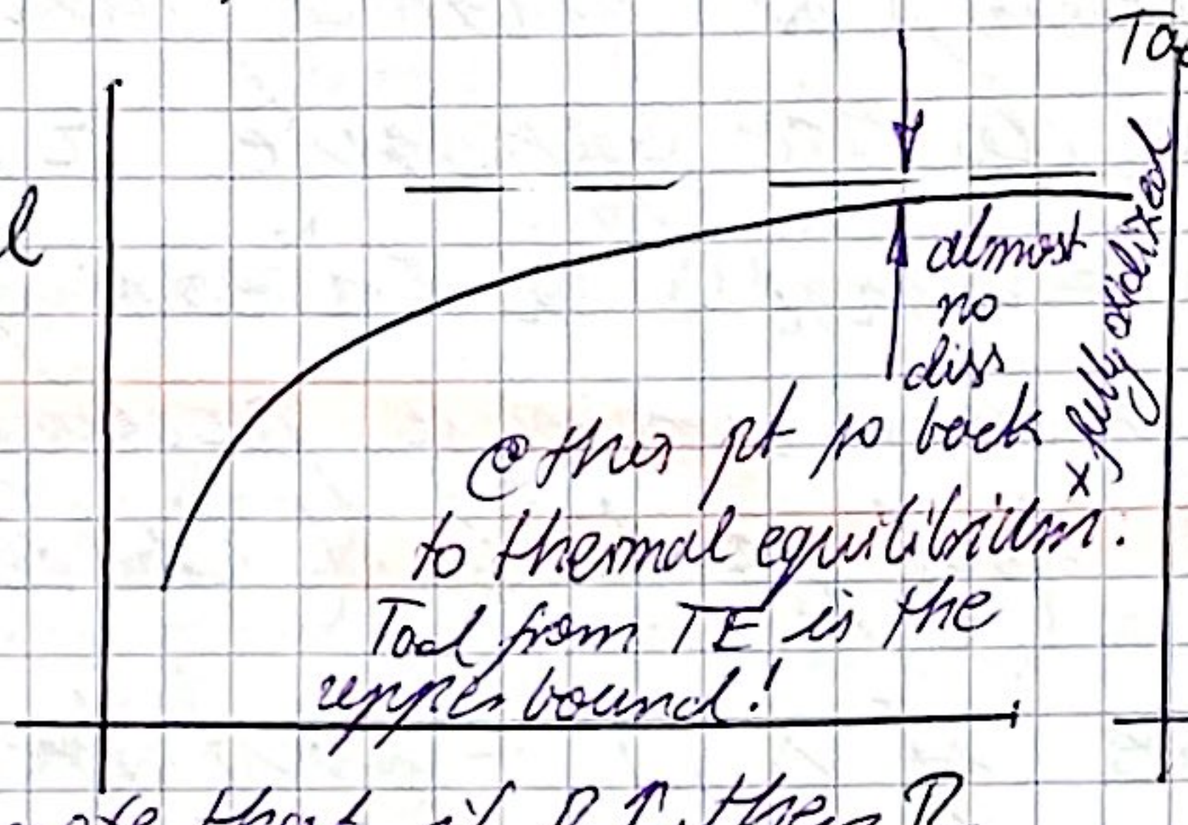
Then if P↑ ⇒ reaction quotient↓. If T=const, then products must increase (so if less moles of products comp to reactents, then shift to products)

c) $\sum \nu > 0$, e.g. dissociation

$$CO_2 \rightleftharpoons CO + \frac{1}{2} O_2$$
(1) (1.5)

If $p \uparrow \Rightarrow$ quotient $\uparrow$, no χ of reactants $\uparrow$ to keep $K_p = const$ @ $T = const$

(~~more products. Have more reactants if $p \uparrow$~~)

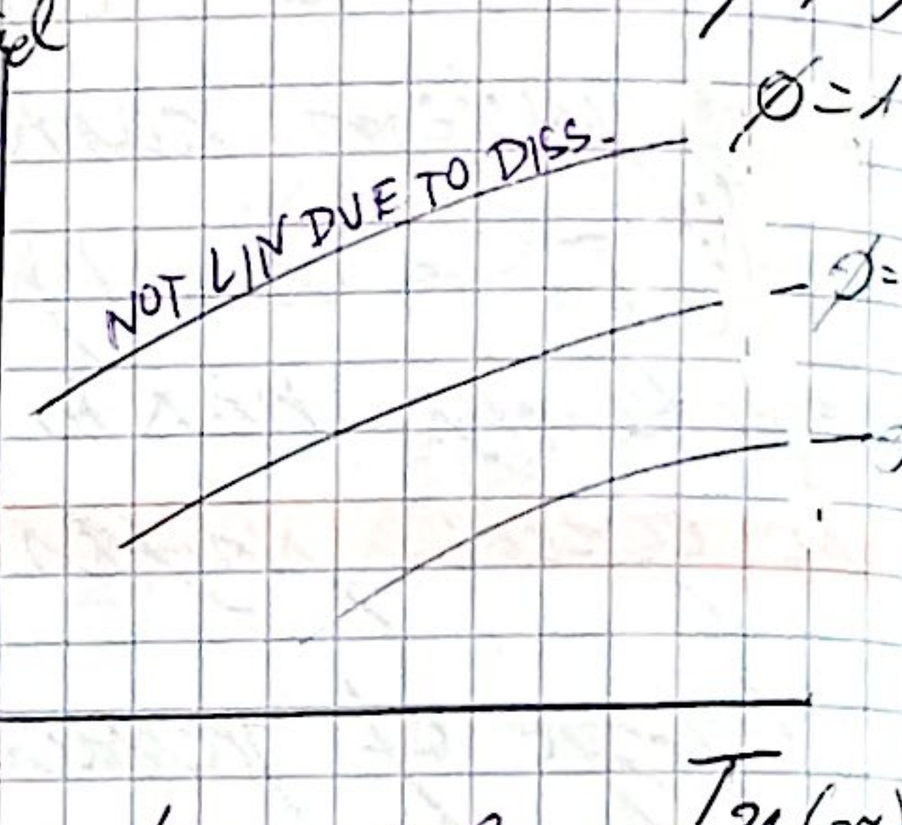


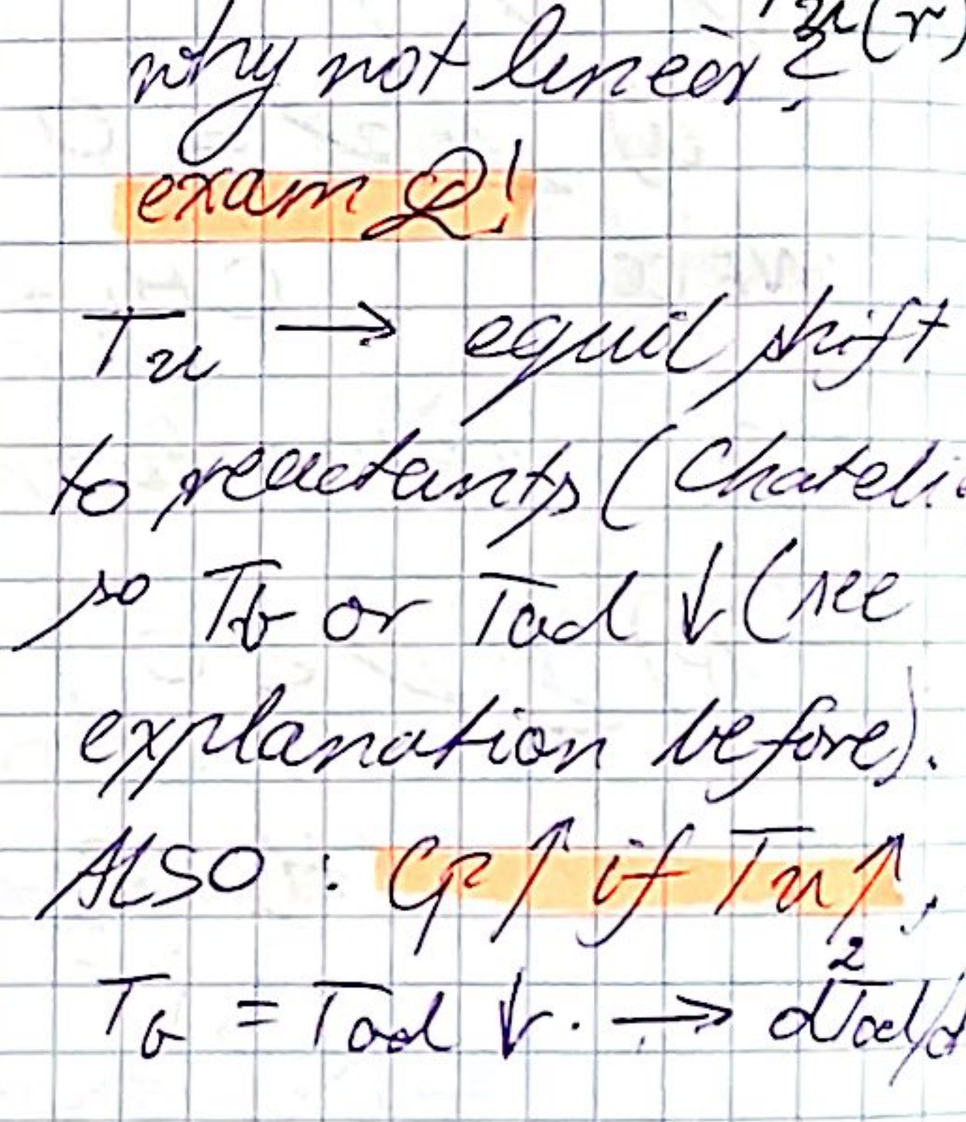
note that if $p \uparrow$, then R both a) & c) say shift towards exothermic, so $T_{ad} \downarrow \Rightarrow$ consistent

only if $\sum \nu = 0$, then $T_{ad} \neq T_{ad}(p)$

Physically, @ higher p represses dissociation so more exothermic so $T_{ad} \uparrow$

Also, less en. is stolen to break dissociation bonds so more sensible enthalpy.





why not linear?

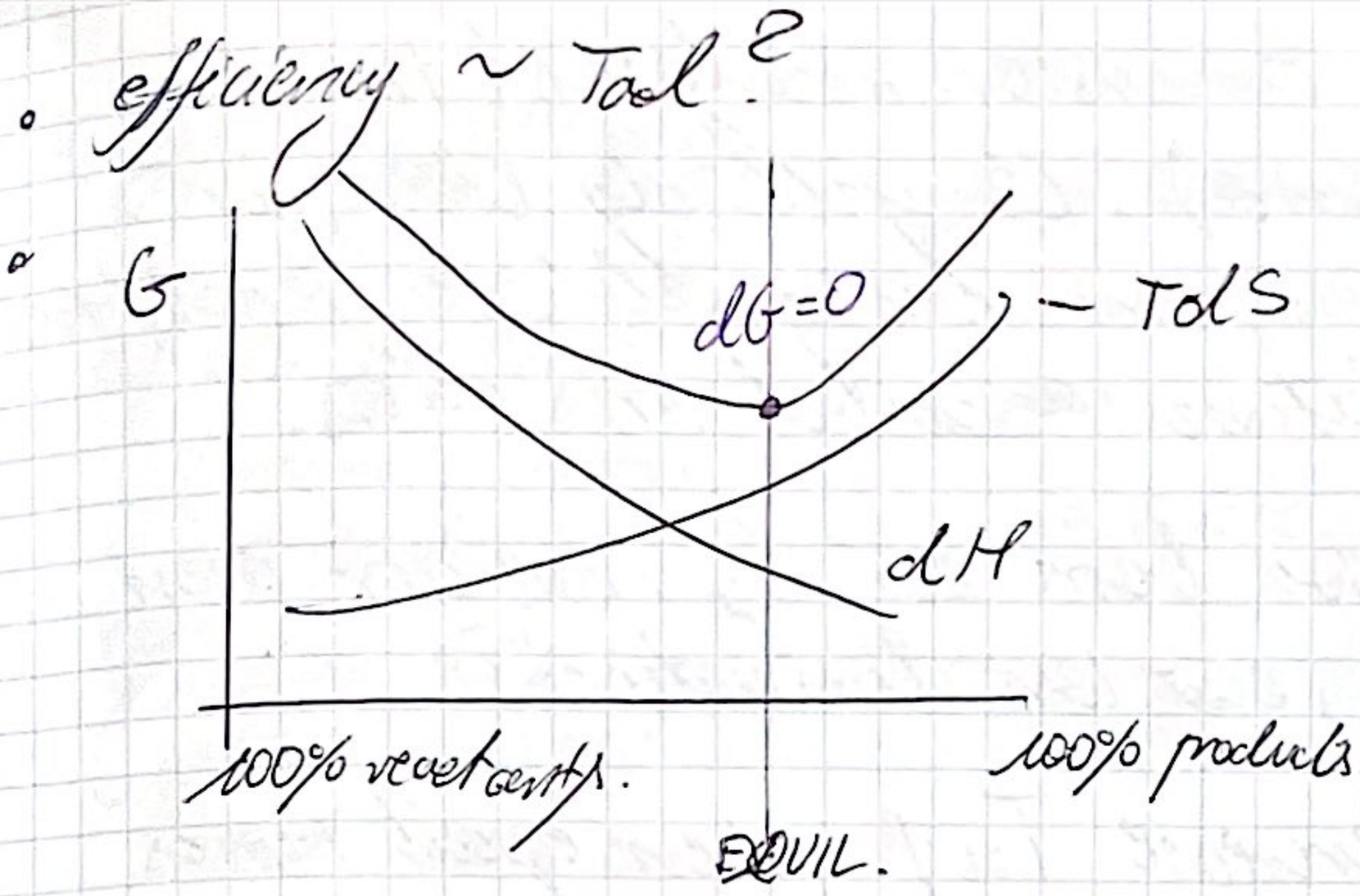
exam Q!

$T_{ad} \rightarrow$ equil shift to reactants (Chatelier) so T_b or $T_{ad} \downarrow$ (see explanation before).

ALSO: GP $\uparrow$ if $T_{ad} \uparrow$, $T_b = T_{ad} \downarrow$. $\rightarrow$ $d T_{ad}/dr$

"Dissociation" reactions are the only cause of chem eq. — they rush / they're also the cause for NOx emissions for fuels which do not contain N

Isothermal eq. so



③ Chem-Kinetics

1. ∘ Enthalpy & heat balance:
   - Useful only if TSFC is of interest
   - Equil chemistry
     - Influence of P & composition can be accounted for
     - assumes ∞-fast, which leads to overprediction of slow species such as NO
     - in reality, the equil assumpt is only good for hydrogen diffusion flames — Not considering N_2 rxns.
     - we need to account for correct time scales thru f & reverse chemical rates → Chem. Kin
     - You DO NOT assume complete cx.
   - Chem Kin
     - when influence of P, T & time becomes

important. Emission analysis (thru residence time). Complex bcs, for a general fuel, in being able to forecast rns correct rns & associated rns rates.

2. ◦ "If you burn in O_2, not air, then T_f, cuz less dissociations"?

◦ "If increase T_{in}, then equil moves fwd reactants"

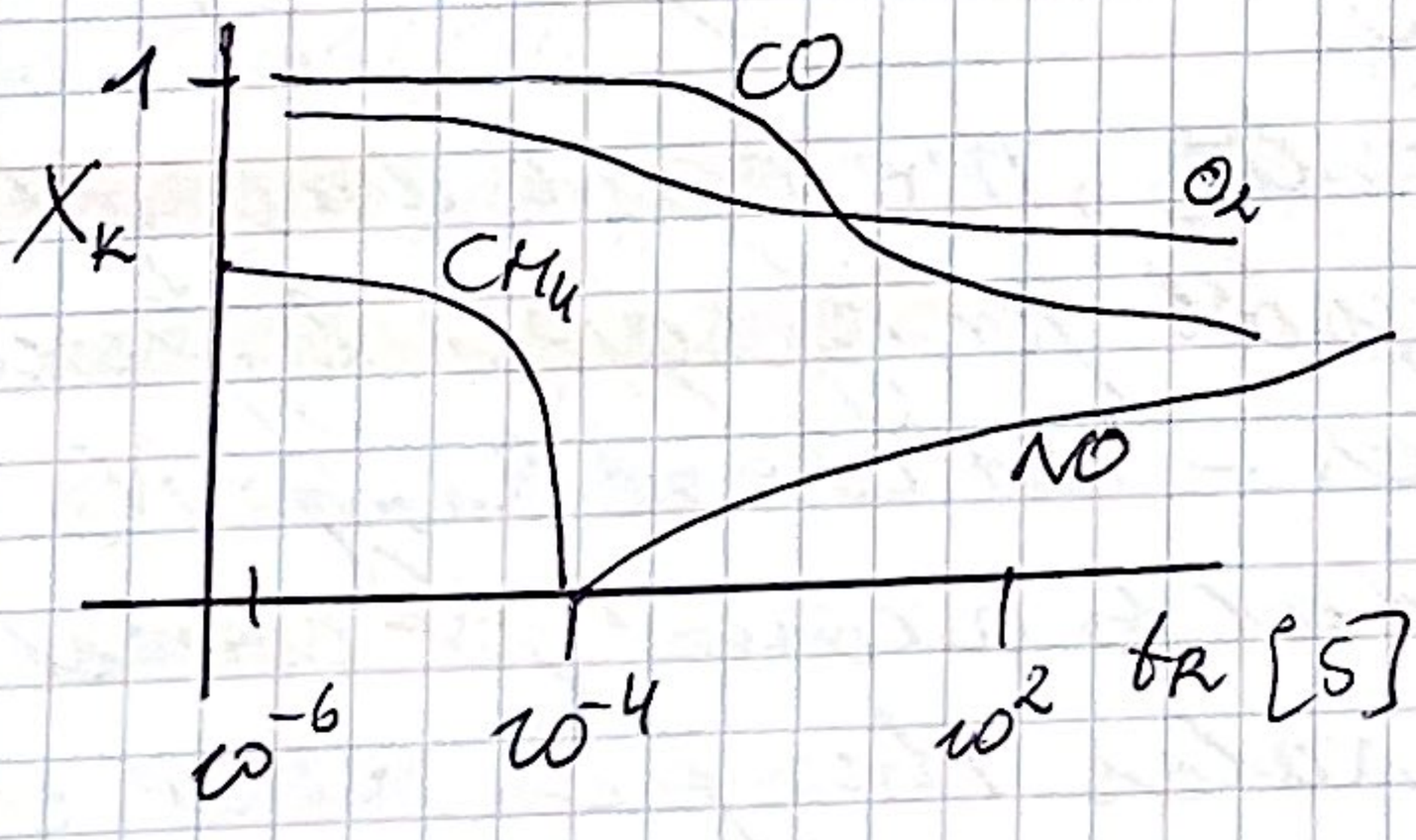
◦ "Chemeq is useful only when rns are fast (constant enough)"

◦ "If you use lean, then can't use chemeq anymore, or when NO is produced" WHY? cuz of t_R >>?

• $t_R^{NO} \sim 10^{-2}$ [s]

• $t_R \propto$ CC volume.

3.



4. Types of systems

a) OD systems (mimic stirred reactors),
they assume that the system is homog & closed. Assume mixing time ≪ chemical time)
→ explosions: = ∃ fast pct of rns (radicals) that exponentially grow in time ≠ DETONATION
→ auto-ignition

b) 1D, 2D, 3D systems
(transport phenomena important)
(chemical time ≈ or ≫ mixin' time)
→ deflagration = speeds are subsonic, ~~isochoric~~ isobaric
→ detonation = SW + CC, not treated here

5. Chem of Chemkin

Branch of chemistry dealing with the study of rates of chem rns & their governing factors:

∴ [X], T, P, catalysts / inhibitors, if ∃ radiation &/or other secondary mechanisms

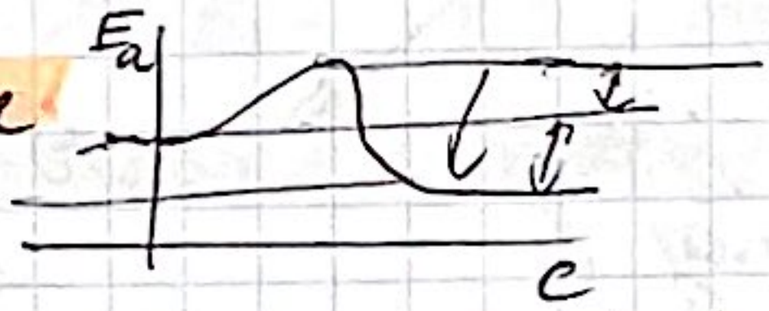
It's used to develop & predict the rn mechs for reacting flows

Rn paths are very complex & out of scope

Rate of rn $\dot{\omega}_{jk} := \frac{d Y_{jk}}{dt}$ and recall the properties it has. (Q: etc)

6 In kinetics, to predict speeds, you need to predict how many bonds are broken & with what probability.

Collision is a necessary but not sufficient criterion for combustion. Eg. H_2 & I_2 undergo about 10^{20} collisions per sec, but only one in 10^{13} is a successful rxn. The likelihood is determined by orientation & Ea



According to Boltzmann, the probability of a molecule having this threshold energy is proportional to:

$$P \sim \exp\{-E_a/RoT\}$$

ONLY VALID IF YOU DO HAVE A COLLISION!

In 1888 Arrhenius posed that molecules must possess a minimum energy to react Ea. According to the collision model, this energy comes from KE of colliding molecules. Upon collision, this energy is used to stretch / bend, break bond leading to chem rxn. The KE is used to change the pot energy of the molecule.

$$RR := \pm \frac{d}{dt}[X_k]$$

To model properly the reaction rate, your model needs to take into account @least the following:

- Collision frequency, Z_{AB}
- Steric orientation (factor), S
- Temp
- Ea

Then:

$$RR = Z_{AB}\, S \exp\left[-E_a/R_0 T\right]$$

From kinetic theory of gases, the collision freq is:

$$Z_{AB} = [X_A][X_B] N^2 \sigma_{AB}^2 \sqrt{8\pi k_B T / m_R}$$

- $\sigma_{AB} := \frac{1}{2}(\sigma_A + \sigma_B)$ = avg diam of the molecules
- m_R = reduced mass = $\frac{m_A m_B}{m_a + m_B}$

More generally, compactly:

$$RR_j = [X_A][X_B] \cdot K_{f,j}(T), \text{ where}$$

$$K_{f,j}(T) = A_j T^{B_j} e^{-E_a/R_0 T}$$ ← modified Arrhenius eqn.

(non-modified: $A_j \exp[-E_a/RT]$)

The main task of modern chemistry is to find $K_{f,j}(T)$! (difficult)

In general, for elementary reactions, you have the following **Rate laws**:

		Rate = k * :
Unimolecular	$A \longrightarrow P$	$[X_A]$
Bi	$A + A \rightarrow P$	$[X_A]^2$
Bi	$A + B \rightarrow P$	$[X_A][X_B]$
Ter	$A + A + A \rightarrow P$	$[X_A]^3$
Ter	$A + A + B \rightarrow P$	$[X_A]^2[X_B]$
Ter	$A + B + C \rightarrow P$	$[X_A][X_B][X_3]$

usually only @ high P.

Or:

$$RR_j = k_{c_j} \prod_k^{N\text{species in rn } j} [X_k]^{\nu_k'}$$

Law of Mass Action

↓ acc from kinetic theory!

$RR \propto [\,]$

(only for specific, j-th rn)

to know the overall $RR = \sum_j RR_j$.

So, to reiterate, given:

$$\nu_a' A + \nu_b' B \rightleftharpoons \nu_c'' C + \nu_D'' D$$

define fwd rn rate

$$RR_{f_{ij}} = -\frac{d}{dt}[X_A] = -\frac{d}{dt}[X_B] =$$

$$= k_{f_{ij}} \cdot [X_A]^{\nu_a'} [X_B]^{\nu_b'}$$

and reverse rn rate

$$RR_{r_{ij}} = +\frac{d}{dt}[X_C] = +\frac{d}{dt}[X_D] =$$

$$= k_{r_{ij}} \cdot [X_C]^{\nu_C''} [X_D]^{\nu_D''}$$

note: $RR_j > 0$ always

So that: $\mathcal{Q}_j = RR_{f_{ij}} - RR_{r_{ij}}$ (or $\mathcal{Q}_j = 0$)

& @ equilibrium: $RR_{f_{ij}} = RR_{r_{ij}}$, so

$$k_{f_{ij}} \prod_{r \in R}^{N_{REACTANTS}} [X_r]^{\nu_r'} = k_{r_{ij}} \prod_{p \in P}^{N_{PRODS}} [X_p]^{\nu_p''}$$

or in one common set:

$$\frac{k_{f_{ij}}}{k_{r_{ij}}} = \prod_k^{NPUN_R} [X_k]^{\nu_k} \left\{ = \frac{[X_C]^{\nu_C''} [X_D]^{\nu_D''}}{[X_A]^{\nu_A'} [X_B]^{\nu_B'}} \right]$$

and the reaction quotient is thus equal to the constant $K_{c,j} := \frac{K_{f,j}}{K_{r,j}}$ called the equilibrium constant.

So, simply, @ equil:

$$\boxed{K_{c,j} = \prod_{k}^{N} [X_k]^{\nu_{kj}}}$$

2. Reaction order. RO is specific to not only j but also r or f. So we may speak of RO for the tuple $(j, r|f)$. Then, RO is defined as the sum

$$RO_{f,j} = \sum_{r \in R} \nu_r'$$

$$RO_{r,j} = \sum_{p \in P} \nu_p''$$

Importance & interpretation. Consider a reaction A, B, C, D, where $\nu_B', \nu_D'' \to 0$ (empty to A & D). Then by def:

$$RR_{f,j} = -\frac{d}{dt}[X_A]$$

but due to law of mass action

$$RR_{f,j} = k[X_A]^{\nu_A'}[X_B]^{\nu_B'} \approx 0, \text{ so}$$

$$= k[X_A]^{\nu_A'}$$

, or ODE

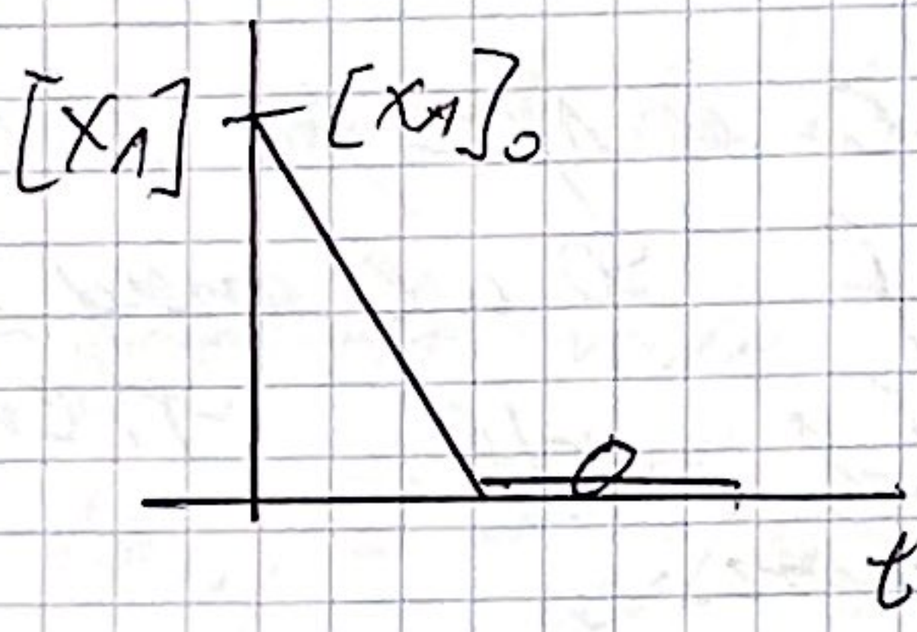
$$\frac{d}{dt}[X_A] = -k[X_A]^{\nu_A'}. \text{ Note that as}$$

then case $RO_{A/J} = \sum_{REP} v_p' = v_A'$

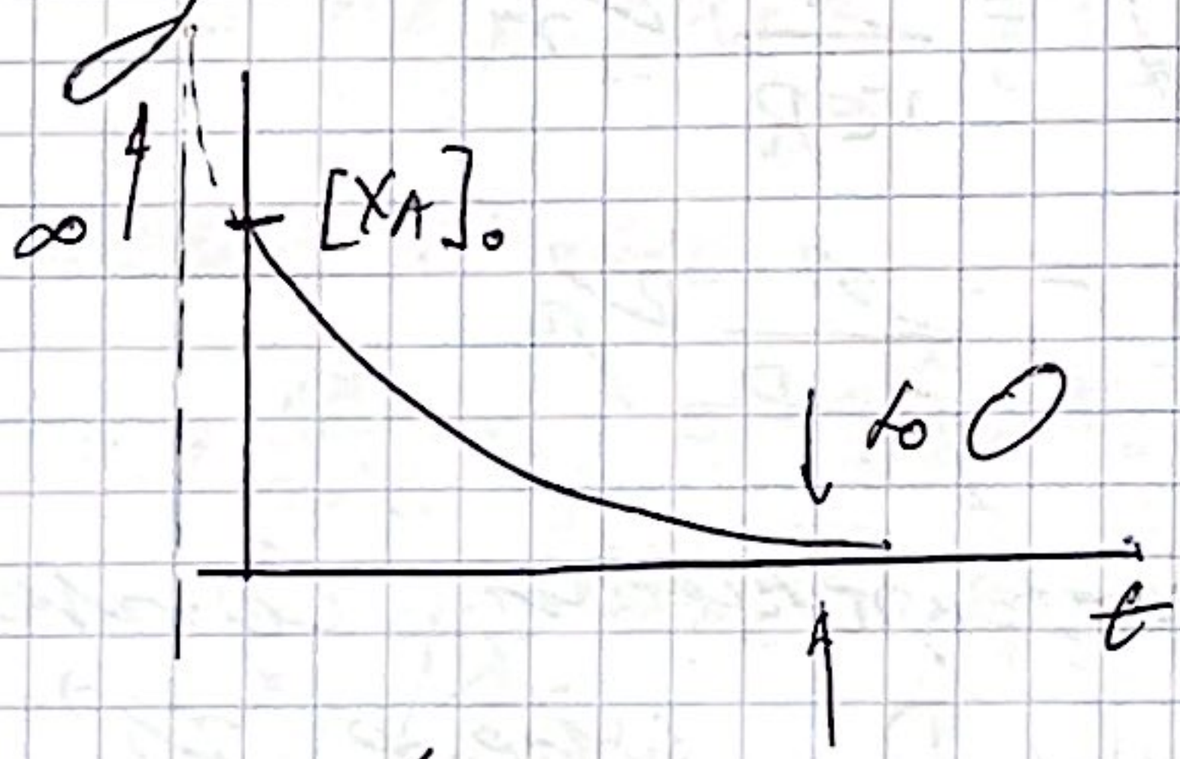
so breakdown to cases:

- $RO = v_A' = 0$: ⟶ happens when you have a catalyst ⟶ then $\frac{d}{dt}[X_A]$ independ of v_A'!

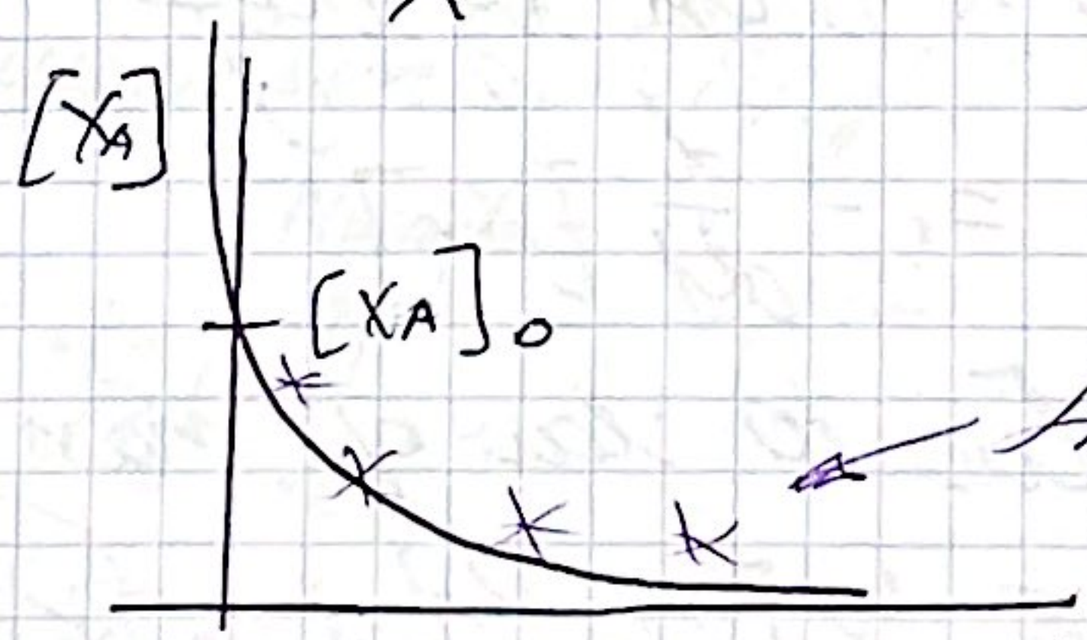
$$\Rightarrow [X_A](t) - [X_A]_0 = -kt \text{ , so } ;$$



- Similarly $RO = 1$: $\ln$:

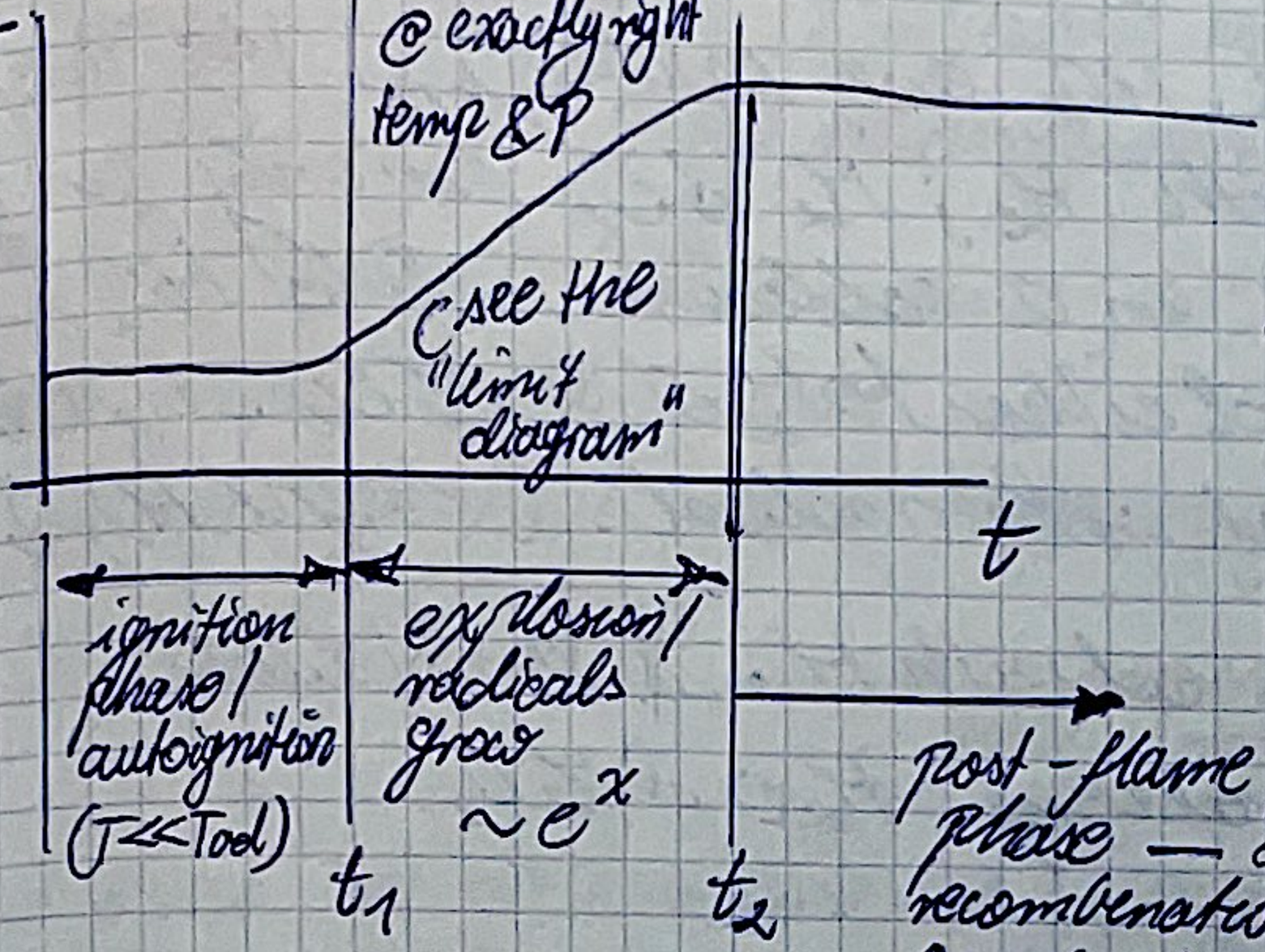


- $RO = 2$: $\frac{1}{x^2}$:



- etc.

Note that ~~...~~ once you have experimental data you can fit data to back-engineer the (equilibrium) constant K_p, K_r, K_c ...



@ exactly right temp & P

(see the "limit diagram"

Take:

$2H_2 + O_2 + 3{,}76N_2 \rightleftharpoons 2H_2O + 3{,}76N_2$



99% of rxns

1) Individuate possible species

- H_2, O_2 — R
- H_2O — P
- O, H, OH, HO_2 — radicals
- H_2O_2, HO_2 — not radicals but unstab. species

– radicals have low E_a, so more reactive than other species

– rxn between radicals are fast b/c extra body is needed to stabilize the product

– stable reactants (species) are only H_2 & O_2

2) Find Elementary rxns. Not everything can react with everything, so only a finite # of rxns possible

- O, OH, HO_2 are oxidants so they can only react with H_2; H_2 & O_2 can only generate O & OH in a collision; while HO_2 can react either to H_2O or H_2O_2. H_2 can only react with radicals (except H), O_2 can only react with H. ∄ bimolecular involving H_2O & H_2O_2.

Bimolecular:

$$H_2 + O \rightarrow OH + H$$
$$H_2 + OH \rightarrow H_2O + H$$
$$H_2 + HO_2 \rightarrow H_2O_2 + H$$
$$H_2 + HO_2 \rightarrow H_2O + OH$$
$$O_2 + H \rightarrow OH + O$$

Dissociation:

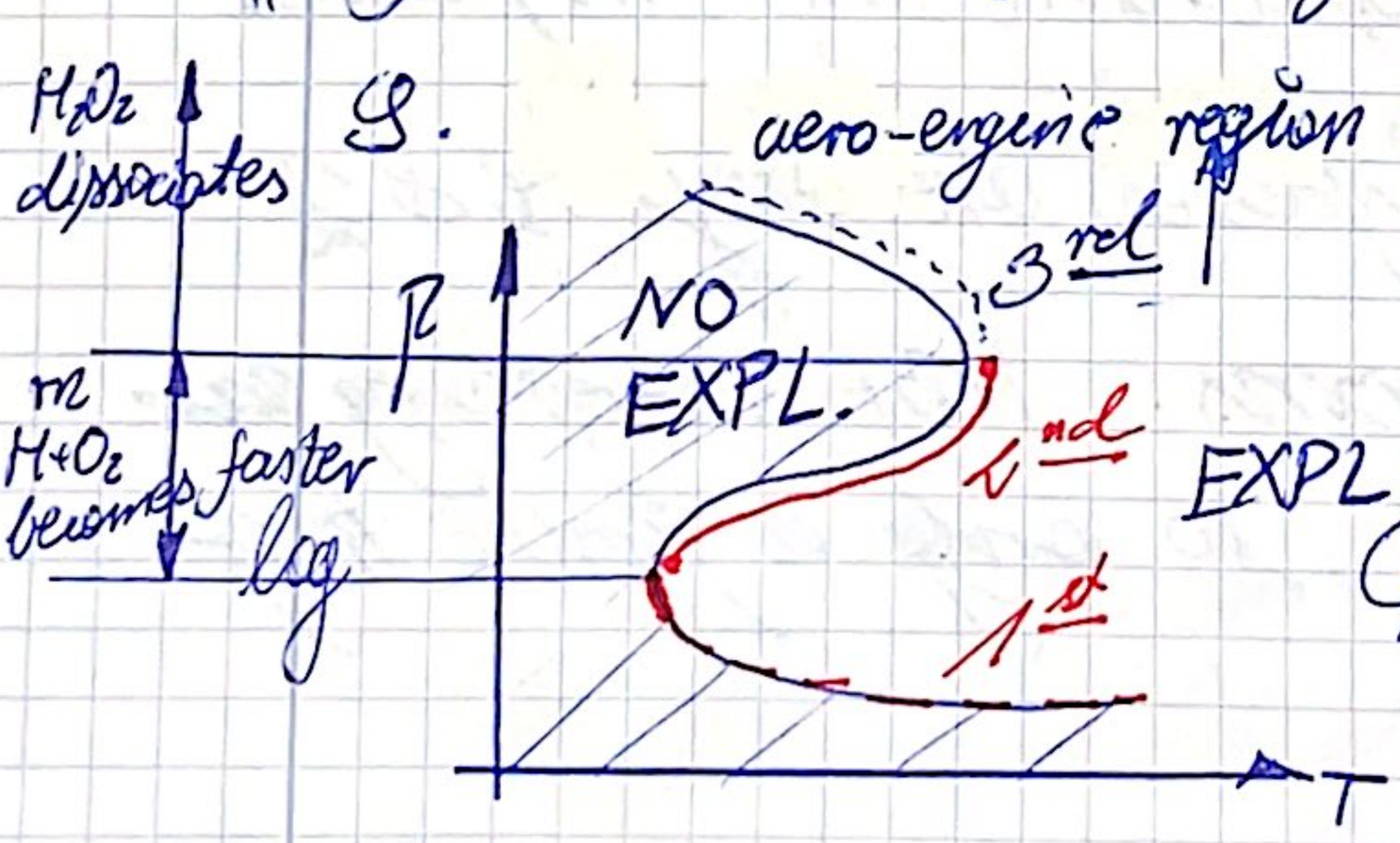
$$M + H_2O_2 \rightarrow 2OH + M$$

Recombination

$$H + H + S \rightarrow H_2 + S$$
$$H + O_2 + M \rightarrow HO_2 + M$$ } only @ high P

(autoignition = Spont. ignition = Self ignition)

3) fuel routes (flux diagram) = fn(T, p)



EXPLOSION LIMITS

$$H_2 + O_2 \rightarrow H_2O + H_2O_2 + \dots$$

EXPLOSION (spontaneous)

→ hypergolic mixture (w/o spark)

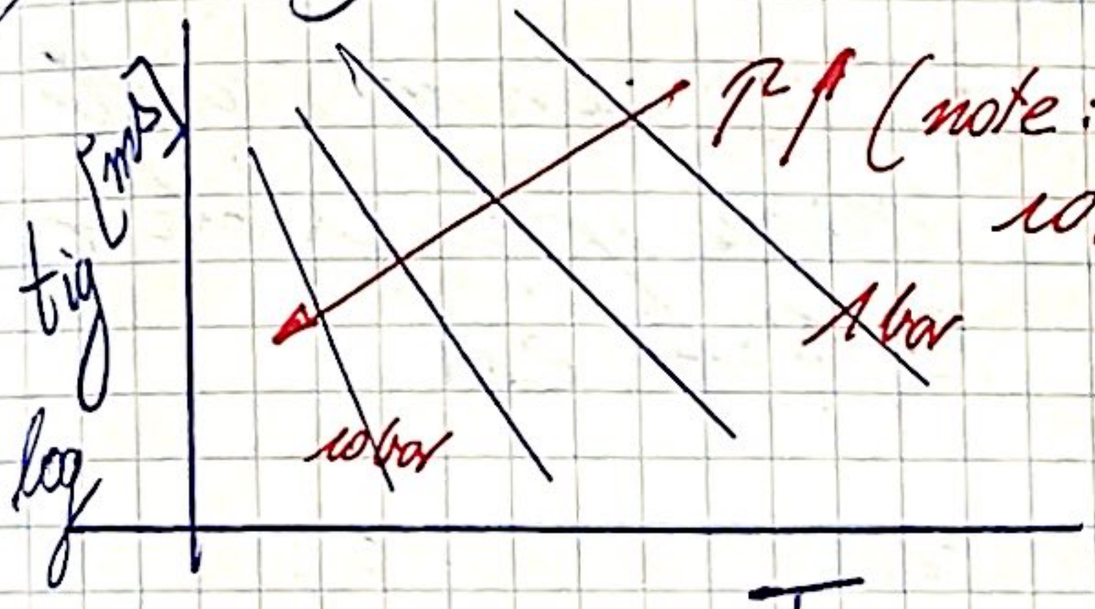
1st limit → p low, T_r also low & matter, the m will not occur. Only recombination occurs

2nd lim → rr will occur, it'll take some time but it will.

3rd lim → rr won't happen, again, but if T_r ↑, it will.

→ note that spark ignition used if not hypergolic; but then it creates ignition kernel

But even if ur mixture is hypergolic, cc won't happen instantaneously. One can study how quickly the rrs get to the point of exp growth of radicals: ignition time! (delay) tig



"Hydrogen has 100M faster tig than other fuels, it can autoignite"

- tig decreases an OOM with each 100K or 2 atm
- tig —11— with $[X_{O_2}]$↑
- Arhenius eqn can be imprecise @ some conditions: tig can increase with T or p (fuels with $C_m H_n$, $m > 4$). — bad if autoignition.

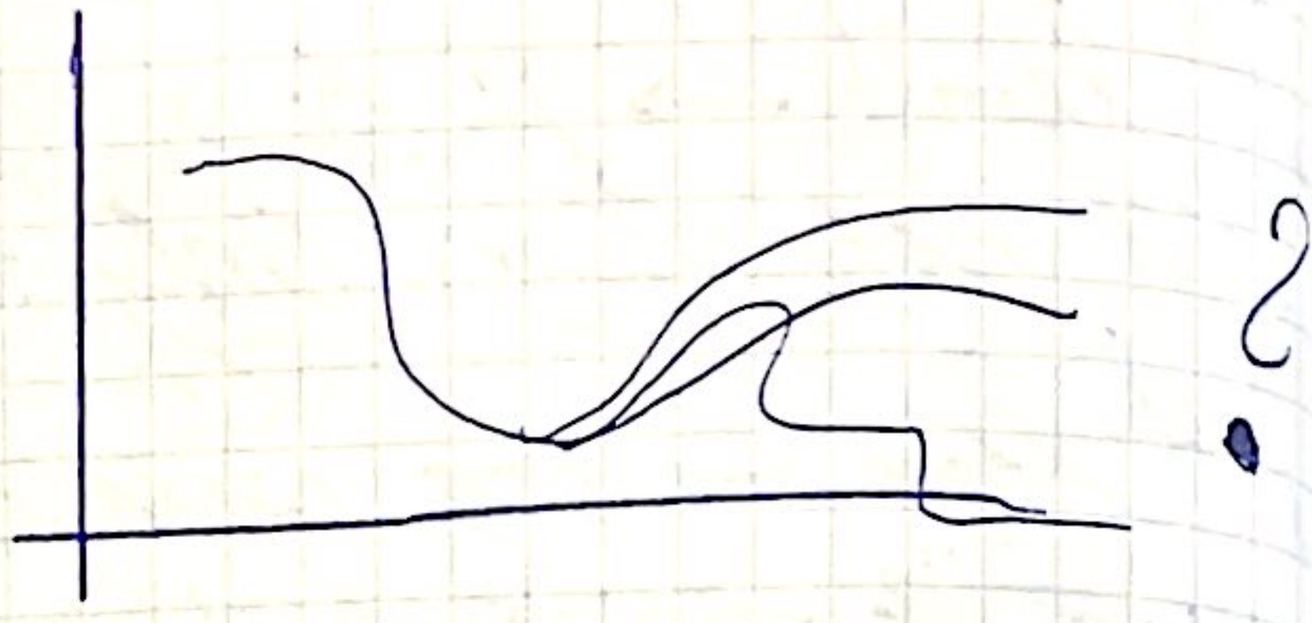
10. NO_x

Formation mechanisms: (that's fuel-NO_x + O in air (if fuel contains N))

Fenimore — Prompt

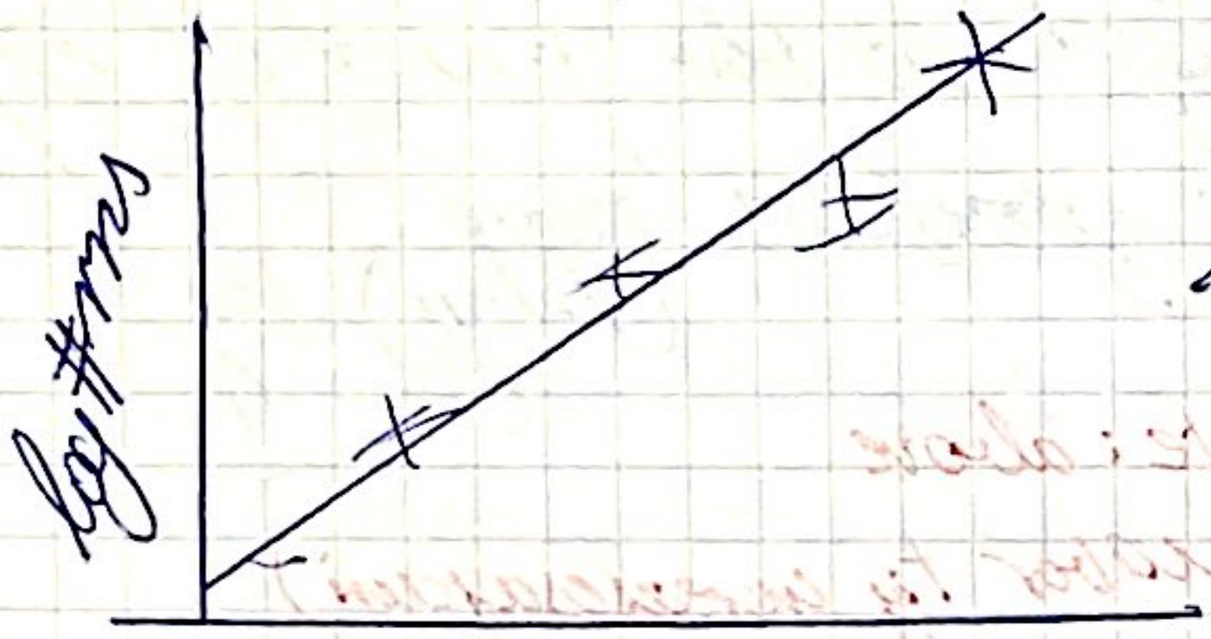
Zeldovich — Thermal (bc N + O from air, needn't have N in fuel)

- Fuel
- NNH Route
- N_2O Route



11. Methane Oxidation
- Gri-Mech-3.0 ~ 54 species & 325 rxns with $(E_a, A_j, B_j) = fn(\phi)$
- If optimized as a whole, selective tuning should not be done

12. Reaction sets



- Uncertainty over completeness for mechanism
- CFD cannot handle many species due to stiffness
- Sensitivity of a mech is a problem
- Ambiguity in model params
- Uncertainty propag into model predictions
- Multiple competing pathways
- Nonlin, non-monotonic trends
- Real fuels have many species

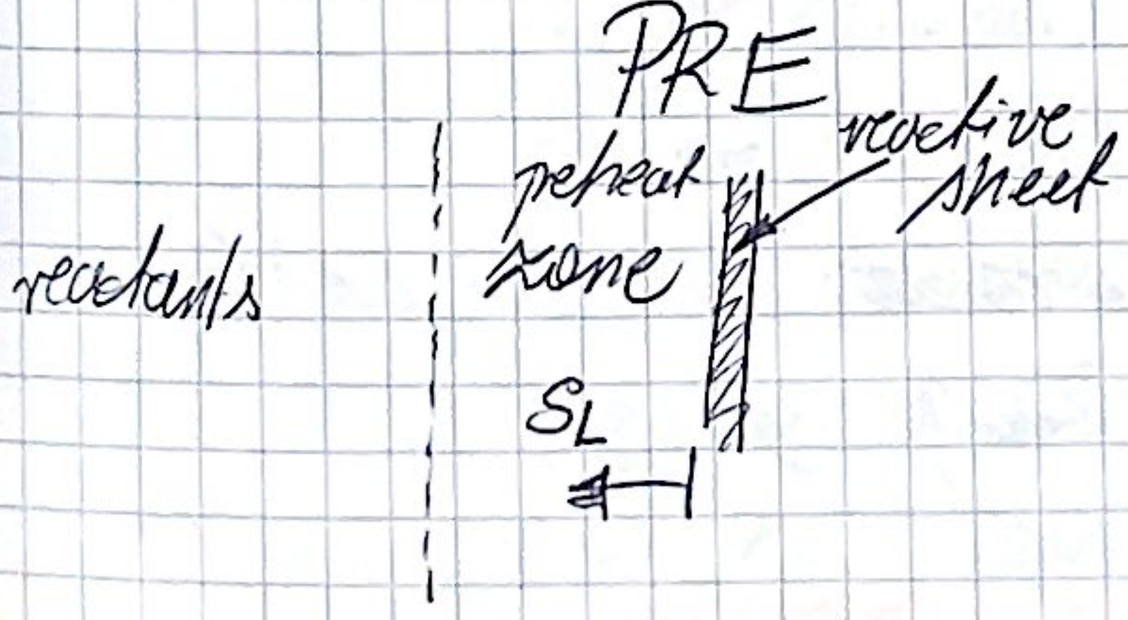
CFD or CHEMISTRY_2
need to balance 'em!

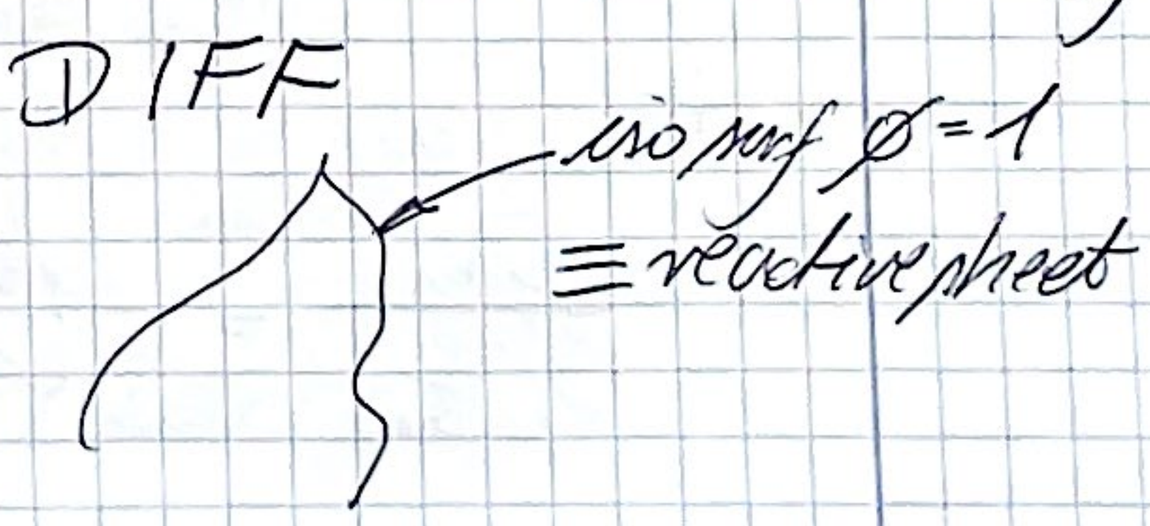
When chemistry can be more important?
— Ignitions & extinction; Emission prediction; Parametric analysis: EGR, mass changes in O. etc.

④ Basics of Combustion

1. **Premixed flames have speed!** Why? If flame is premixed, CC can take place anywhere in the mixture. What limits it is the need to transport heat & radicals from the thin reactive sheet (flame front) into the cold, unburned mixture in front of it. This leads to a propagating front with a clearly defined rate of progress (flame speed) It's determined by: chemical time scale (rate of heat release) & thermal & momentum diffusion — how fast the heat & momentum/radicals leak ahead) ⟶ governed by micro physics (thermo-mom diff)

2. **Diffusion flames don't have speed.** CC can only happen when the two streams mix into stoich-proportions. This is only governed by molecular or turb diff of species across a shear layer. Any motion you observe is only due to external flow motions. ⟶ gound by macro physics (shear layer thickness, turb eddies)





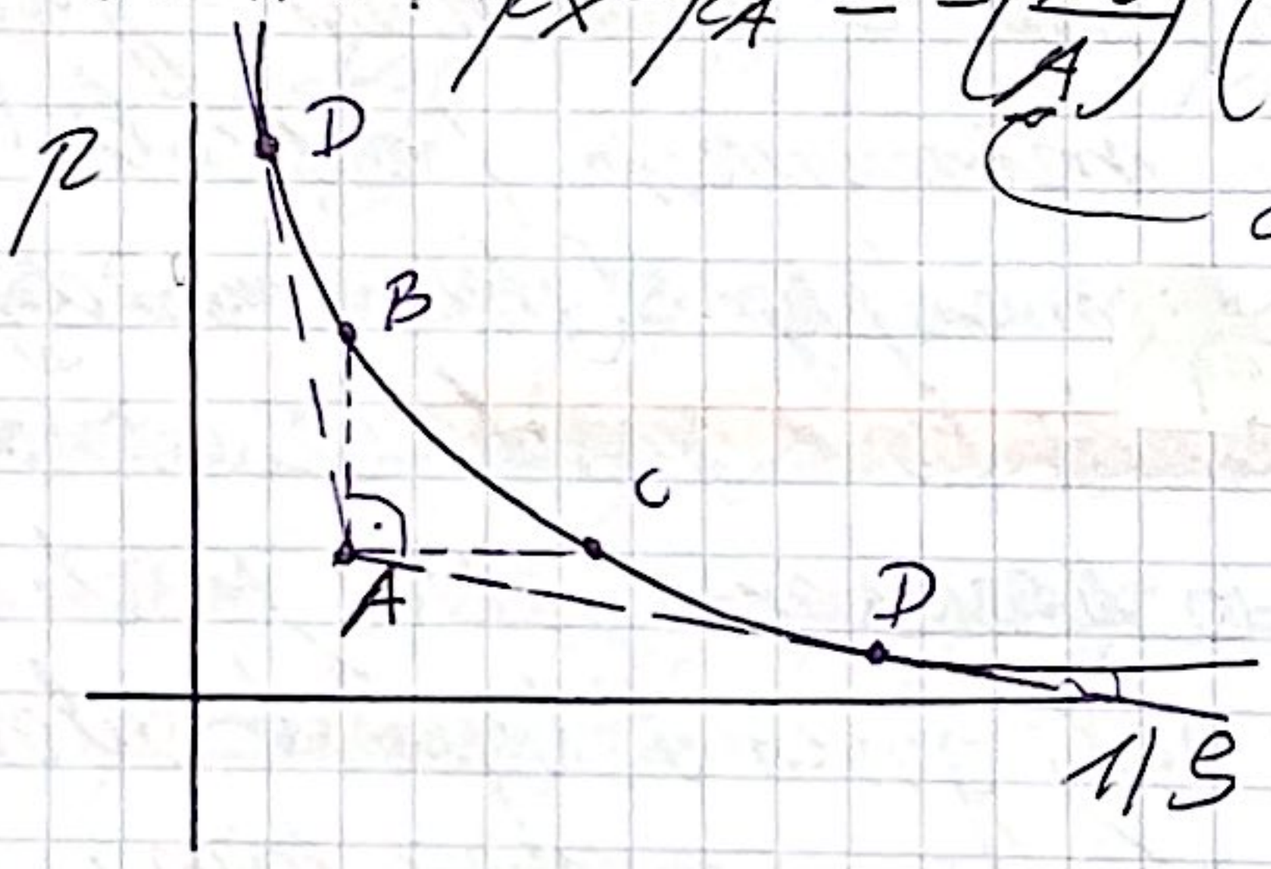
2. Why is appropriate # of radicals necessary (but not sufficient) for cc to occur? Gas-phase hydrocarbon or hydrogen oxidation proceeds mostly thru chain rxns. Radicals are carriers of the chain. If their production rate doesn't @ least balance the loss rate (recombination wall quenching), the chain terminates & reaction freezes. Thus a minimum specific radical concentration is a kinetic requirement. Together with minimum $\dot{q}$'' release rate they're necessary but not suff criteria for cc!

3. Hugoniot curve

mass : $\dot{m}/A = \rho u = const$

mom : $p_x - p_A = -\left(\frac{\dot{m}}{A}\right)^2 \left(\frac{1}{s_x} - \frac{1}{s_A}\right)$

($\left(\frac{\dot{m}}{A}\right)^2$ — const)

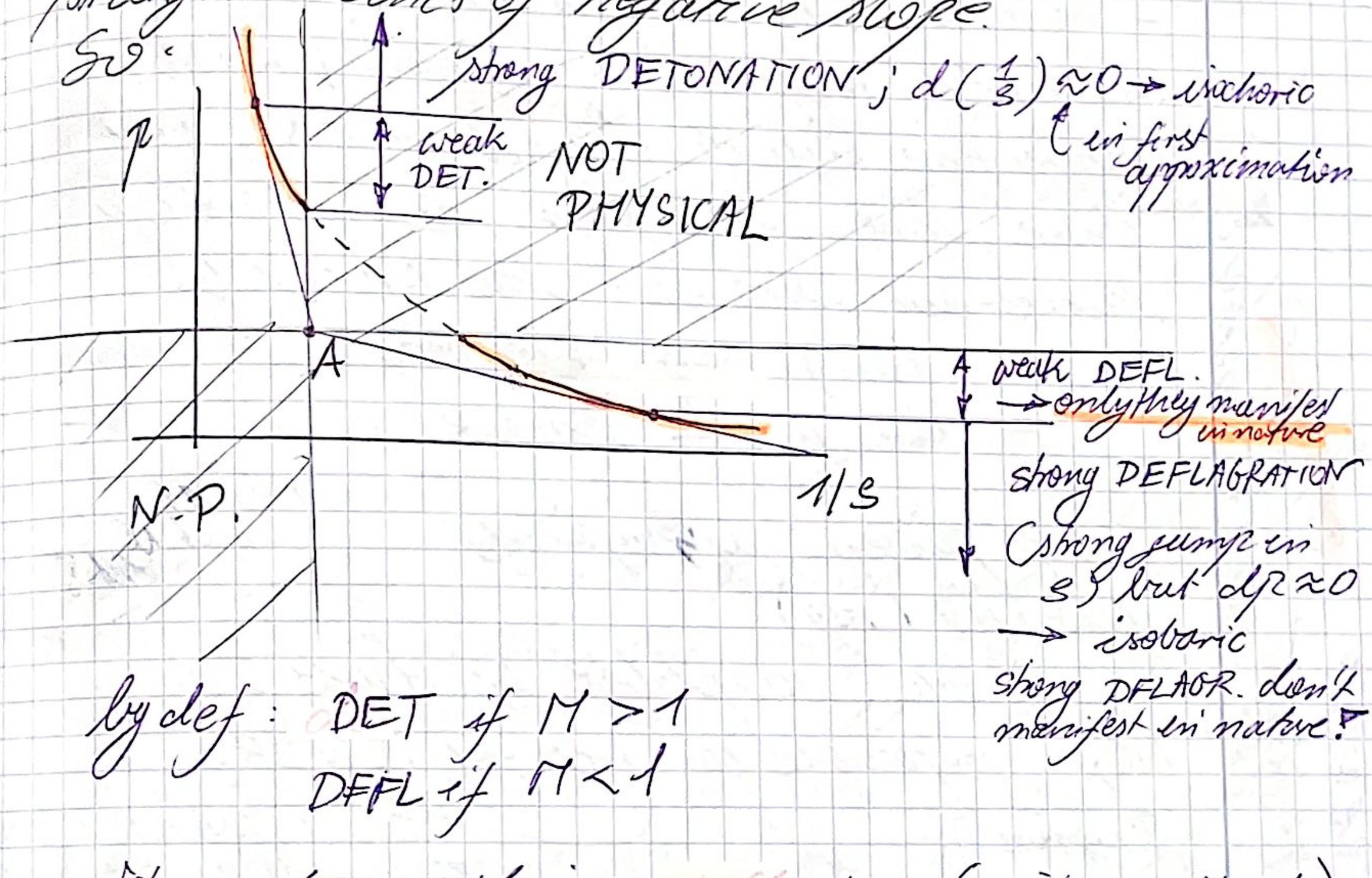


From energy — you'll find that moving A you can only end up, after cc, on the black curve, X.

Take $\partial_{1/s} p$:

$$\frac{\partial p_x}{\partial\left(\frac{1}{s_x}\right)} = -\left(\frac{\dot{m}}{A}\right)^2 = const \text{ (fn of } (\dot{m} \& A) \text{ but only fn of } s)$$

also, the slope is constant & -∞, so can only move from A to X (any on curve) by straight lines of negative slope.



by def: DET if $M > 1$
DFFL if $M < 1$

We're only considering DEFL. here. (isobar + $M < 1$).
DEFL have low propagation speeds & $M \approx 0,3$, so incompressible! But! the density does vary in cc!, even in the limit $M \to 0$. So is it compr or incompr? Incompr! Why? Cuz incompr means s doesn't vary due to p fores, s can & will still vary due to heat release!

4. Some chamber info:

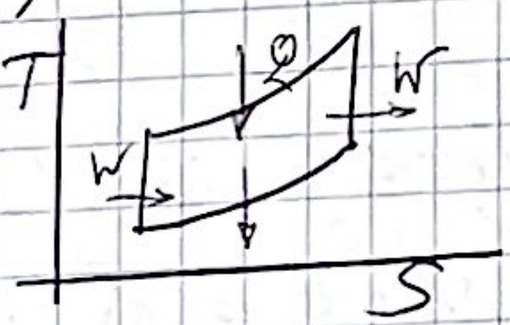
- $M \approx$ const $\approx 0,2 \div 0,3$
- $T_{in} \approx 600 \div 1000$ K
- $v_{in} \approx 200 \div 250$ m/s
- $p_{in} \approx 15 \div 40$ bar
- AFR = 30
- pressure loss $\approx 3 \div 4\%$

- $\eta_{cc} \approx 99,5\%$ >
- flame must be stable
- most critical condition for aeroengines - altitude relight → succesfully restart combustion due to external factors (bird strike, fuel interruption etc). So it's a flame-out condition characterized by:
  - 1/2 low P
  - 1/2 low T
  - 3/4 high $\dot{m}_a$
  - 1/4 low S

- temp pattern appropriate
- low cost (reg)
- CO & UHC acceptable @ LOW power, NO_x acceptable @ HIGH POWER.

might not be right!

- Brayton T



Even if you use premixed (which you do have to control NO_x), there happen stratification → different flame speeds (BAD!)

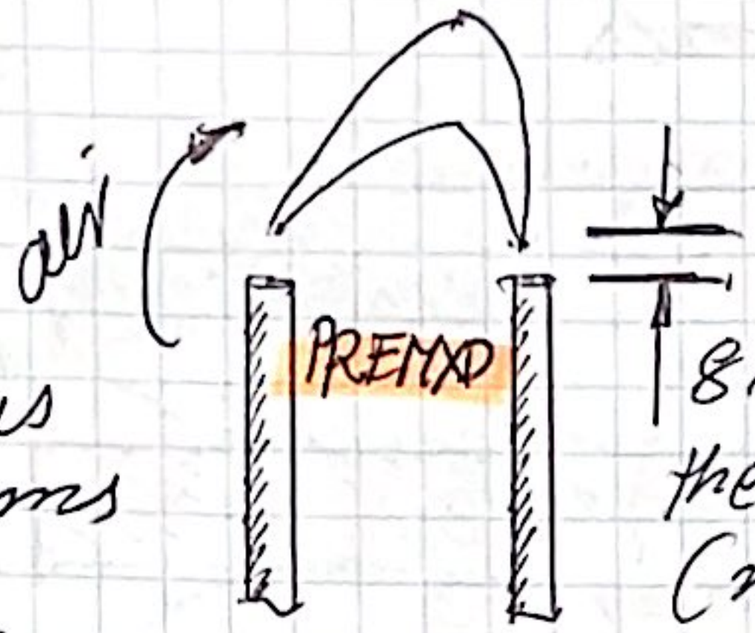
5. TYPES of COMBUSTION

a) Premixed vs Non premixed (:= diffusion) — whether F & O are mixed before combustion at molecular level or not. In premixed systems the reactants are already well premixed. For non-premixed — the reactants are brought together thru transport processes - molecular diffusion & bulk convective motion to a common region where mixing & rxn takes place. In diffusion / non-premixed flame, the position of the flame depends

In premixed flame, the reactants are already mixed & rxn occurs only to the extent that the reactants have diffused & reacted to rxn products.

onthe stoich. ratio — follows $\phi = 1$ ("the stoich. line").

BUNSEN BURNER



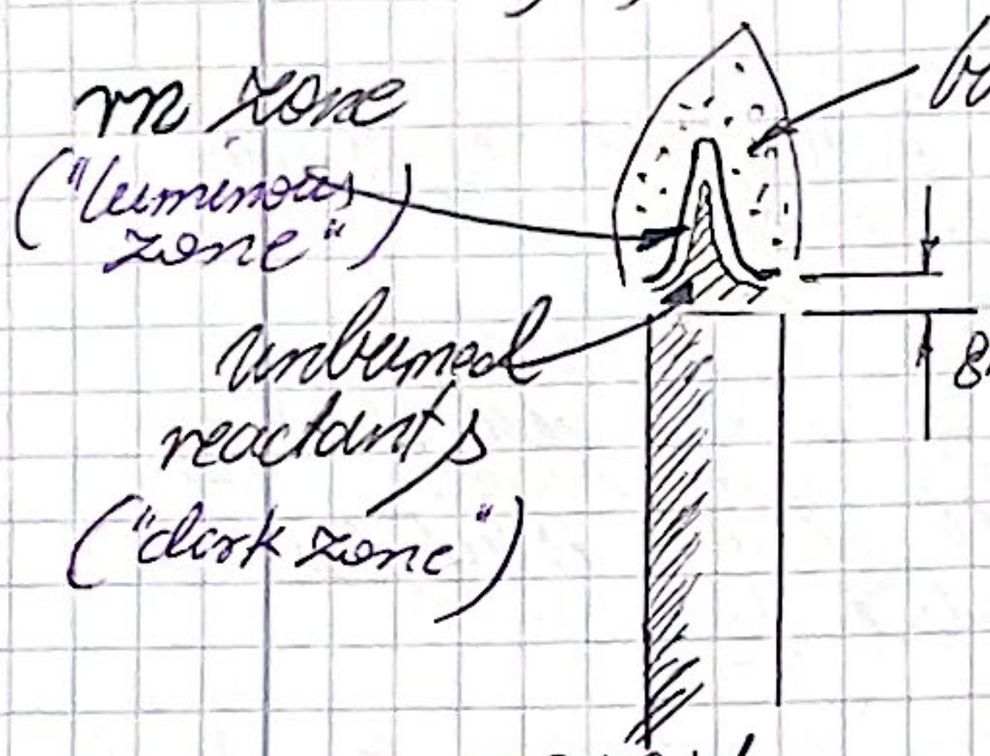
Flame has speed, forms a column.

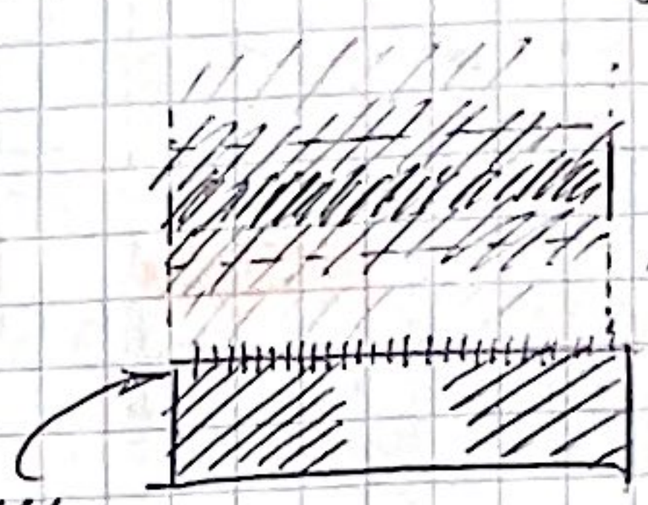
Premixed flames have speed ~ S_L ([X], T, P, diff. rate) and for unique args ∃ unique S_L! (S_L fixed by [X], T, P, DR). Velocity is highest near $\phi = 1$. Flame moves twds reactants. In nature you mostly observe non-premixed (otherwise they would've combusted already). Diff flame more soot (yellow), higher temp ($\phi = 1$), more NO_x (see L5). Premixed are blue due to CH radicals. (see L5). Hydrogen flames are transparent.

b) Terbulent, Laminar. LAM → ∃ distinct lines for the bulk; T → such lines ∄, such that the flow qties "randomly" fluctuate in time. Turb good for mixing and thus has a particularly important impact on diff flames where mixing is essential. However, regardless if L or T, for the rn to take place, the mixing flow MUST take place thru MOLECULAR DIFFUSION.

" In turbulent you don't need to be as precise as in laminar when it comes to chemical reaction rate"

I) laminar premixed (eg. flat flame, burner flame)





flame loses heat to the burner) ⇒ value of S_L is influenced

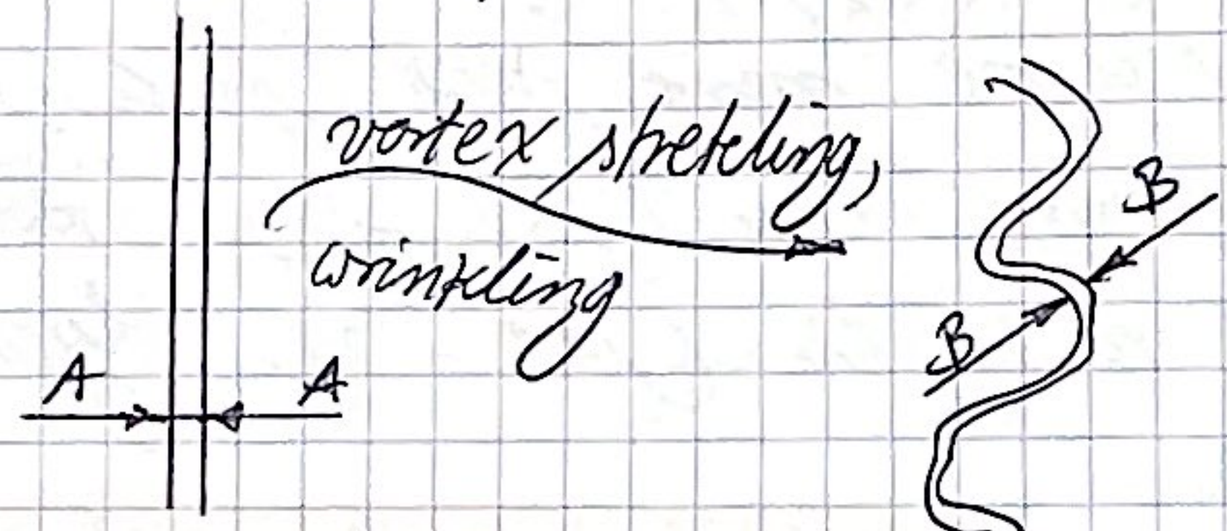
Conical, prem-lam. Flat prem-lam.-burner stabilized.

Stable flame of RICH

- $S_L = -v_u \sin\alpha$

fuels reactants

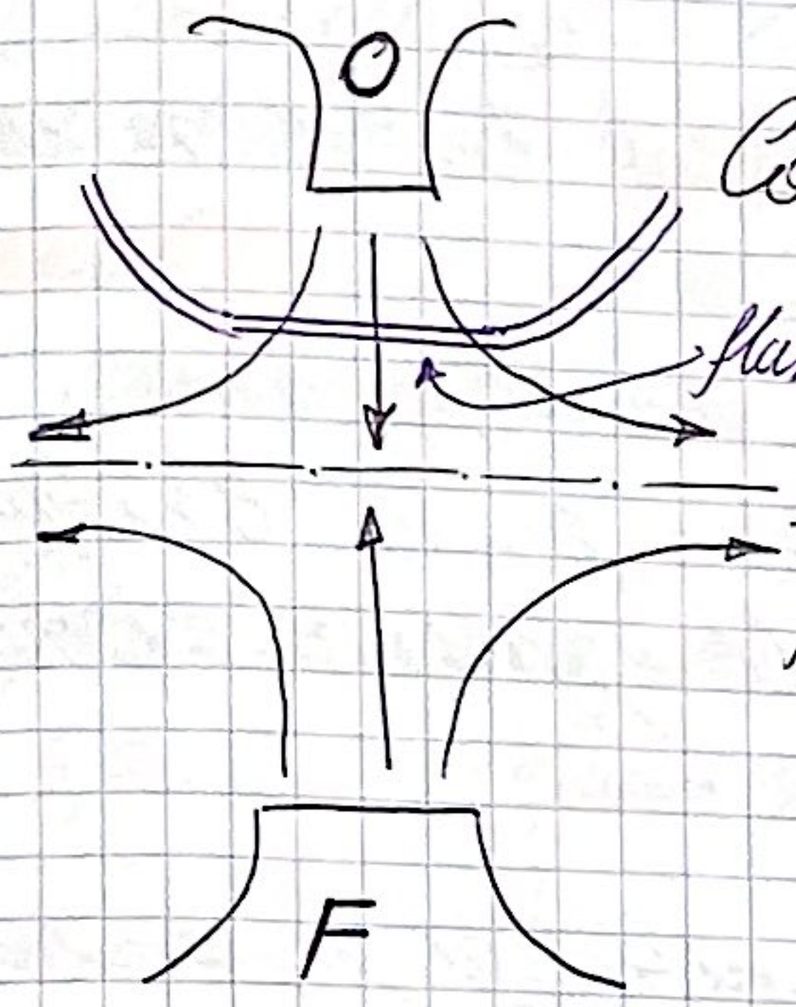
II) turbulent premixed (eg. spark-ignited gasoline engine)



vortex stretching leads to ↑ increased flame surface & flame front disruption (pockets)

Usually, safe to assume the m zone C-S A-A & B-B are visually "similar" which can give many advt (later lectures). This is true as long as scales ie A-A or B-B are smaller than the smallest vortices outside (otherwise chemistry inside affected)

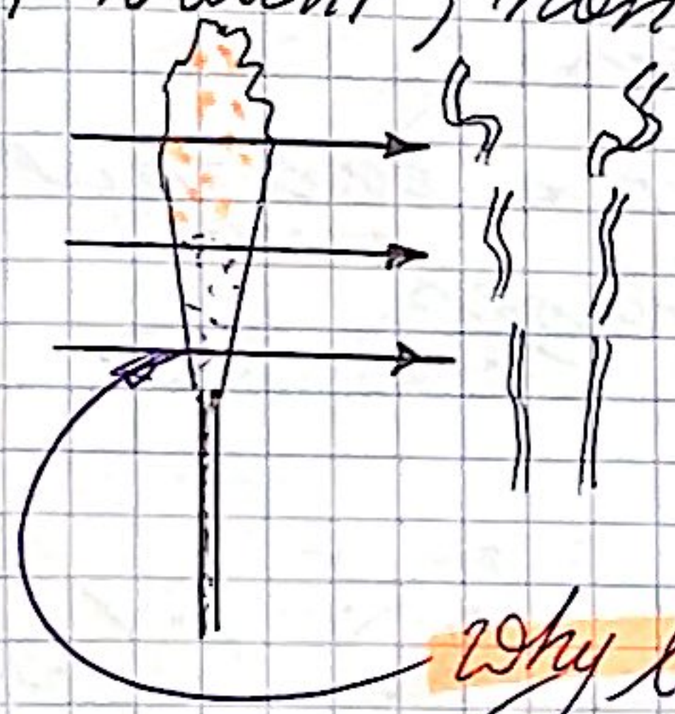
III) laminar, non-premixed (eg. wood fire, candle)



Counterflow-lam-diffusion flame

"Flame is not exactly at $\phi = 1$ due to diffusion"

IV) turbulent, non-premixed (eg. pulverized coal cc, diesel engine, H_2/OX rocket engine)



why blue here?

c) Phase of reactants — homog. / non homog.

Homogeneous is only if the two reactants ÷ O & F — are both at the same time in the same phase — be it liquid or gas — this is one defn.

However, I must define "homog" if O + F (INITIALLY) exist together in the same phase AT LOCATION WHERE RN TAKES PLACE. Since this is often confusing one should say "gas-phase rn" or "surface rn" (coal + oxygen).

more ad a):

PREMIXED:

- reactants are mixed before rn is initiated
- flame propagation resulting from balance of diffusion & rn.
- Initial state can be explosive mixture

NON-PREMIXED:

- Reactants are initially separated
- F&O enter the rn zone as separated streams
- Diffusive transport is essential in mixing the reactants.

PARTIALLY PREMIXED

- Reactants neither pem or non-pem
- <u>local</u> flame propagation (& so speed possible, variable flame speed
- Can occur cuz, e.g.: limitation of mixing device, distributed fuel injection as occuring in spray combustion, due to ign/combdelay (mixing before rn starts)

d) Temporal variation — S or unsteady

e) Role of combustion — propagation or explosion (see L2).

f) Speed → subs, supers (remember $\vec{v}$ and $\vec{u}$ unsimp by def $S_{12} \equiv 0$, but still S_t may not be

g) Heat transfer — adiabatic / non adiabatic
(usually @ walls ∃ heat losses, so not adiabatic! — is that why flame detached from wall? (local extinction?)

h) Convection — natural / forced

i) Gravity — µ-gravity or normal (in µ-g flame is spherical)

j) Spatial dependence — 0D / 1,2,3D systems (see L3)

k) Reaction rate — equilibrium / finite rate

6. Complexity of gaseous combustion
- Laminar: complex diffusion poperties
- Turbulent: wide range of temi & length scales
- Chemistry: # species, # rns, time & lengthscales
- Thermal radiation
- Soot
- Strong coupling of TD-chem pops

(5) Experimental Combustion I

1. Fuel by def is an element ~~accepting~~ donating e^-'s,
Oxidizer ⟵ " ——— " accepts —" —

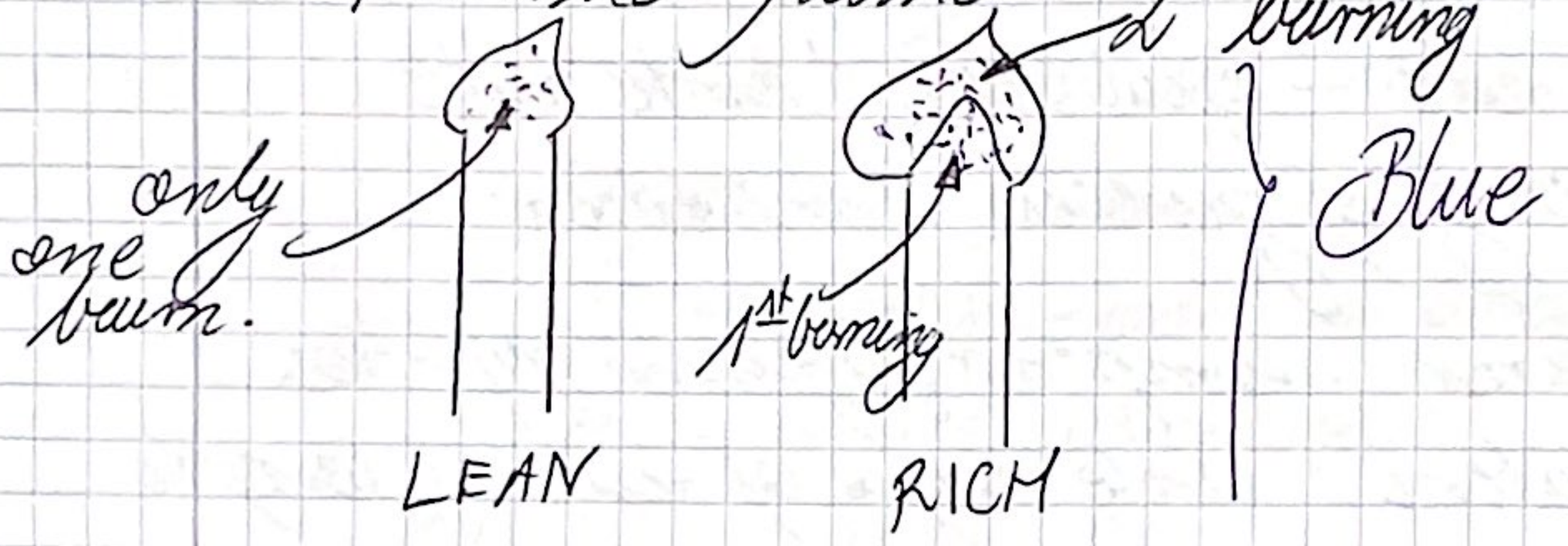
The measure for that is electronegativity — more el-one more pulls elsto itself. Thus, Oxygen is not always an oxidizer! ($E[O] = 3{,}5$, $E[F] = 4$)

2. Types of fuels (& oxidizers)

- gaseous: methane, propane
- liquid: SAF (=kerosene but bio-sourced), kerosene, LPG
- solid: coal, coke, wood

Oxidizer is almost always air or pure oxygen.

3. Premixed flames



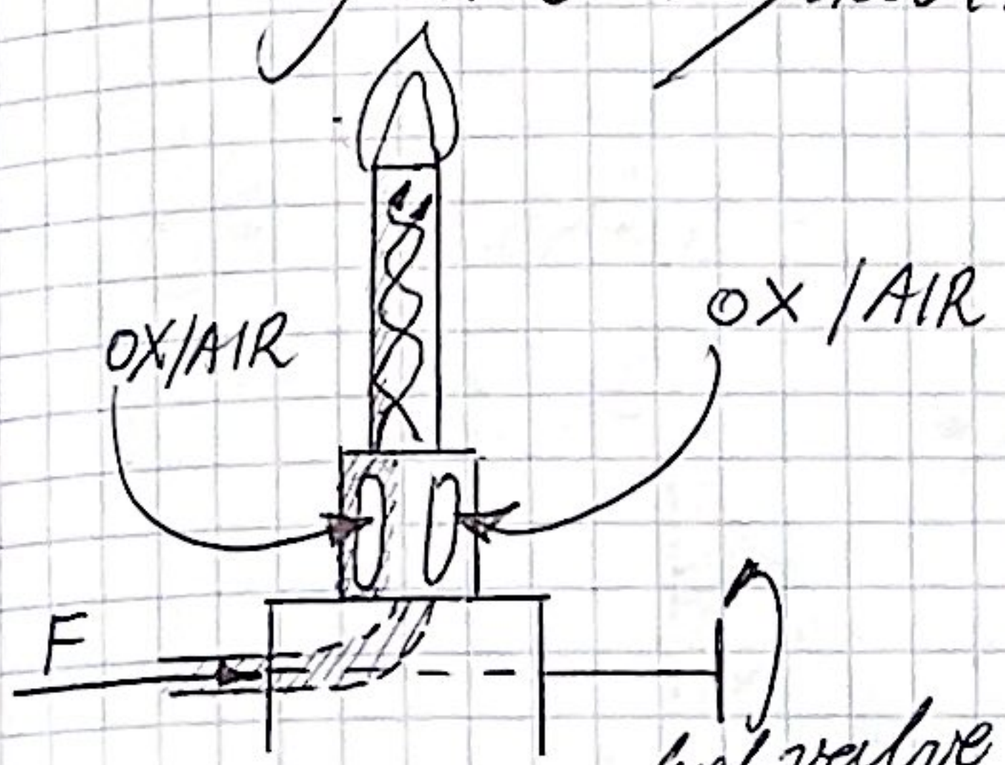
- F+O are well mixed @ molecular level before combustion
- combustion is initiated from a spark or a pilot flame that propagates into unburned mixture
- not common in nature
- less emissions (both soot, NO_x)
- less stable — if T too high, may spontaneously ignite

4. Bunsen burner

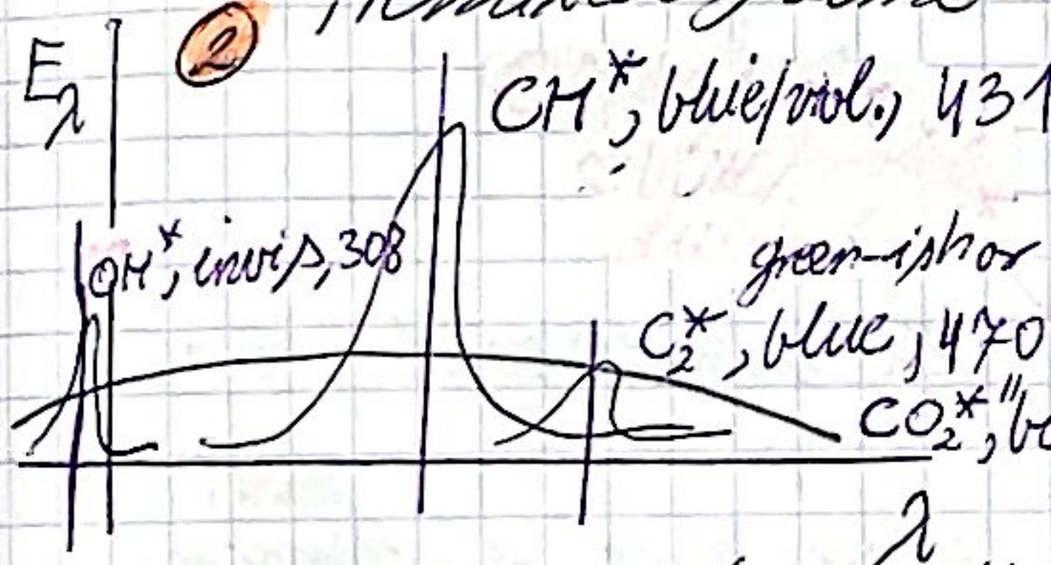
- classical device to generate laminar premixed flames.

- mixing chamber must be long enough to generate a homog. premixed gas

- flame is stabilized on the burner rim



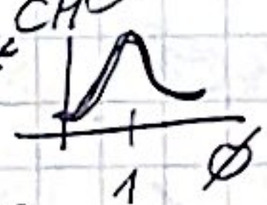
Premixed flame



much less soot (virtually none if $\phi \leq 1$), so → = Δtemp = cont, electron excitation.

chemilum dominates:

1 peak @ 431 nm is due to CH* (absent if H_2 = fuel)



, $CH^* \sim T \approx \phi$

2 peak @ 308 nm is OH* (λ_{vi} = 283 nm, tho)

(not en visible spectrum:

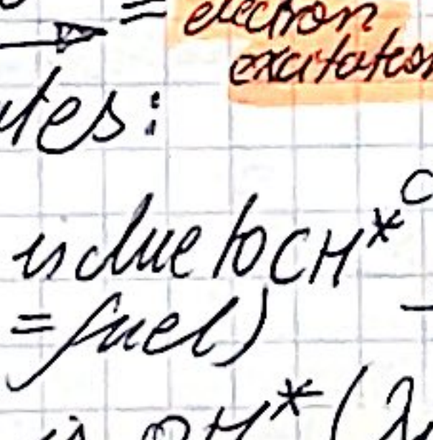
vi's = 380 ÷ 780 nm) (both fuels)

3 peak @ 470 nm is C_2^* (absent en H_2 = fuel)

$C_2^* \sim$ excess carbon

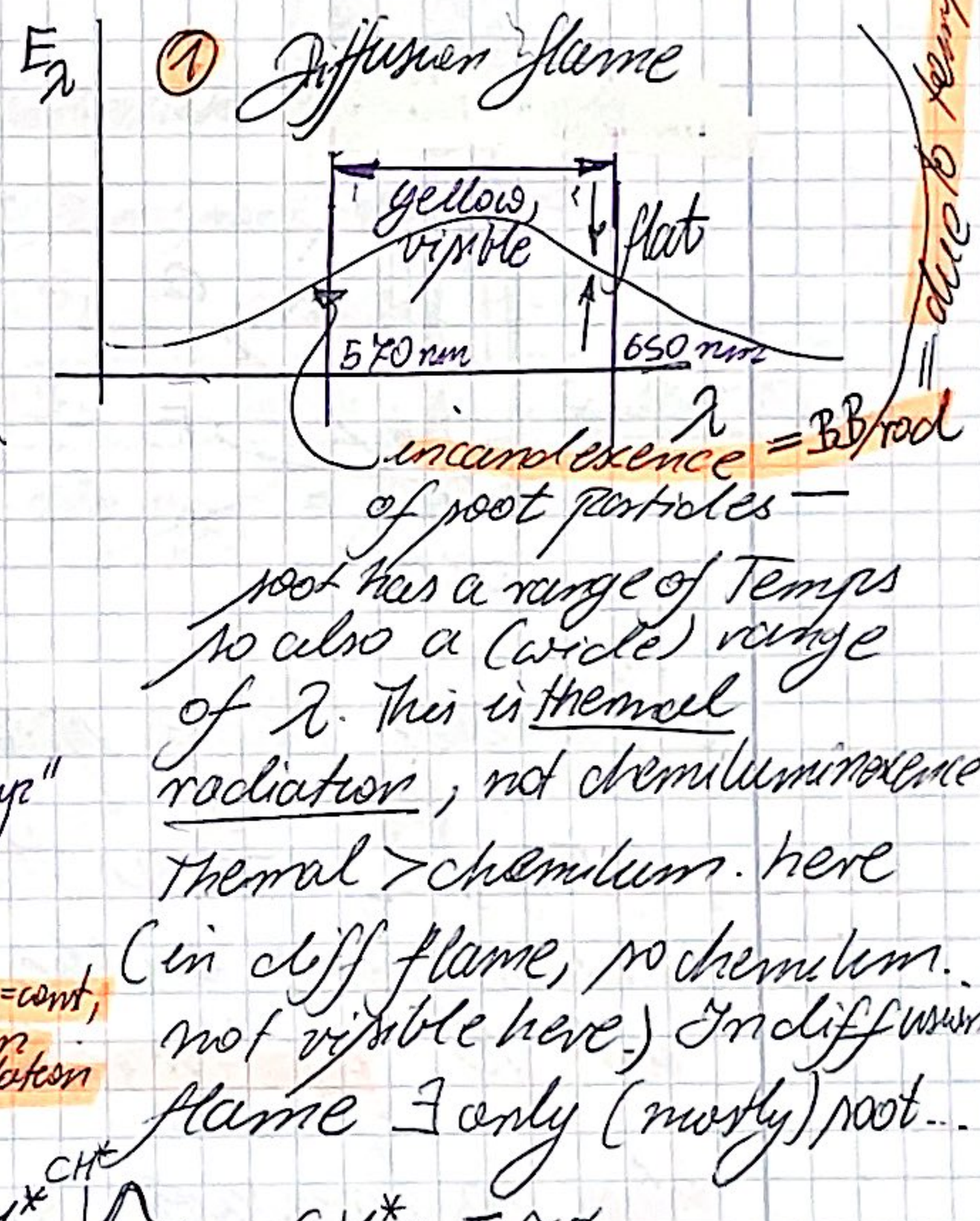
↳ "very rich flames look green-ish"

4 bump is CO_2^*



$CO_2^* \sim$ excess carbon

Spectrum's:

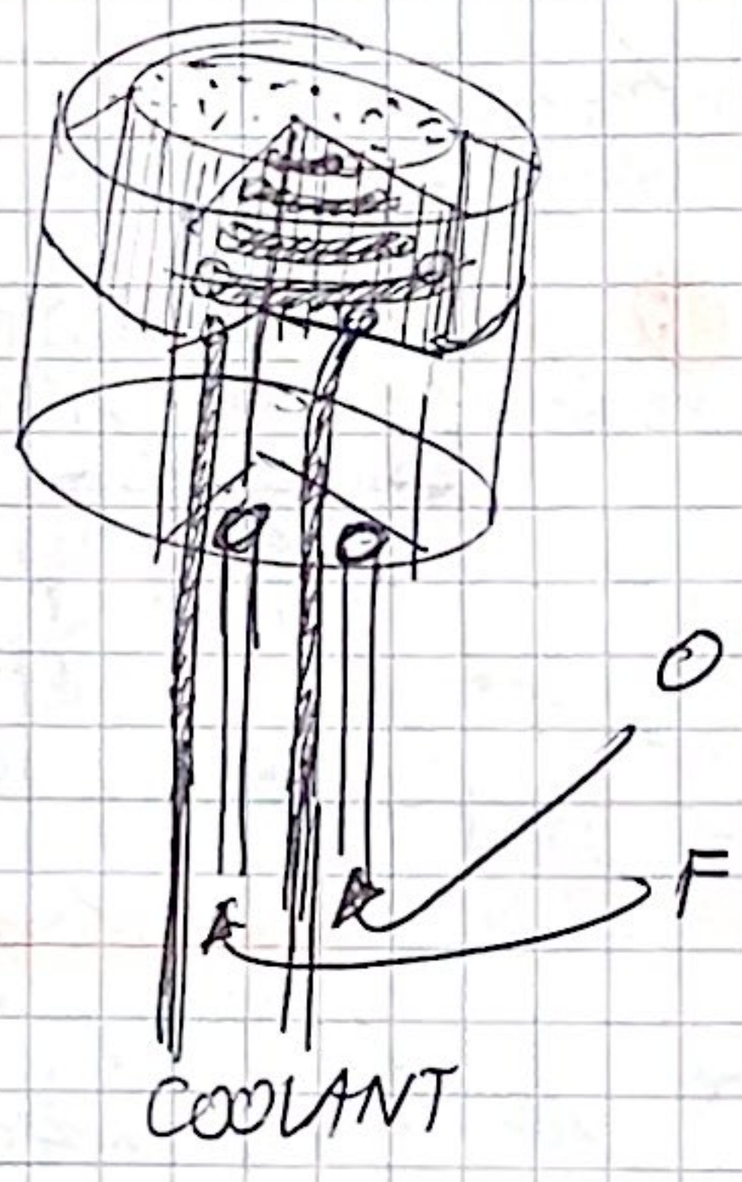


of soot particles —

soot has a range of Temps so also a (circle) range of λ. This is thermal radiation, not chemiluminescence.

thermal > chemilum. here (in diff flame, so chemilum. not visible here.) In diffusion flame ∃ only (mostly) soot...

5. Flat flame burner – McKenna Burner
– generates laminar premixed flame,
highly repeatable, reliable – reference
flame in research
– flame is stabilized on mesh



6. Laminar Flame speed Measurements

LFS, S_L) $\triangleq$ as the velocity of a laminar flame front in the direction $\perp$ to itself wrt to unburned mixture

How to measure S_L?

1) Stationary methods: flame front remains stationary in space (R & flame in opposite dirs)
1 Bunsen Burner
2 Flat flame Burner

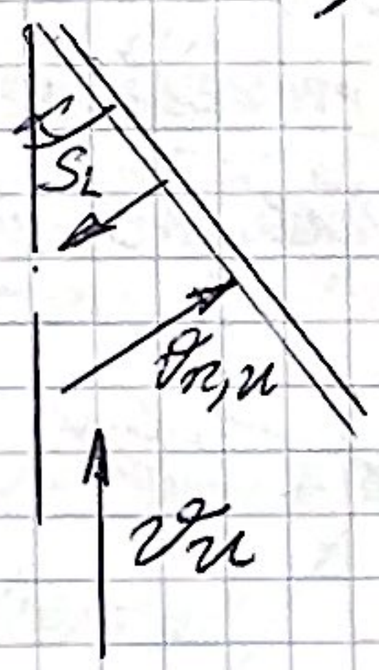
II) Propagation methods : flame front propagates cst same final conditions in space (reactants stationary, flame moves thru space)

1 - tube method

2 - combustion bomb

In practice :

I) 1 :



• Kinematics balance

$v_{flame\ front}/u = 0$

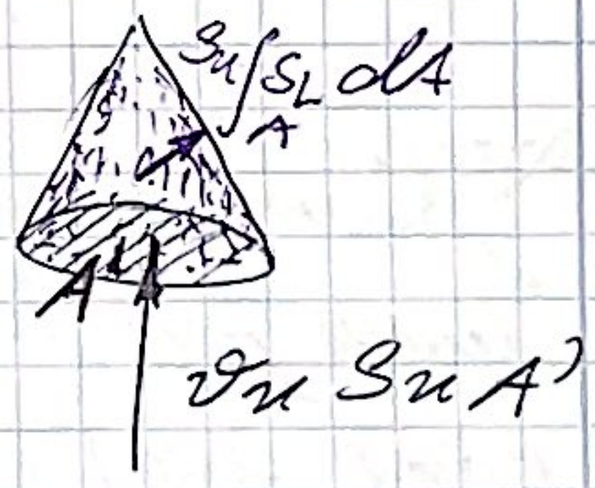
$S_L - v_n/u = 0$

$\boxed{S_L = v_{n,u} = v_u \sin\alpha}$

$v_{n,u}/v_u = \sin\alpha$

• or mass flux balance :

assume $S = S_u = const$ inside the cone :



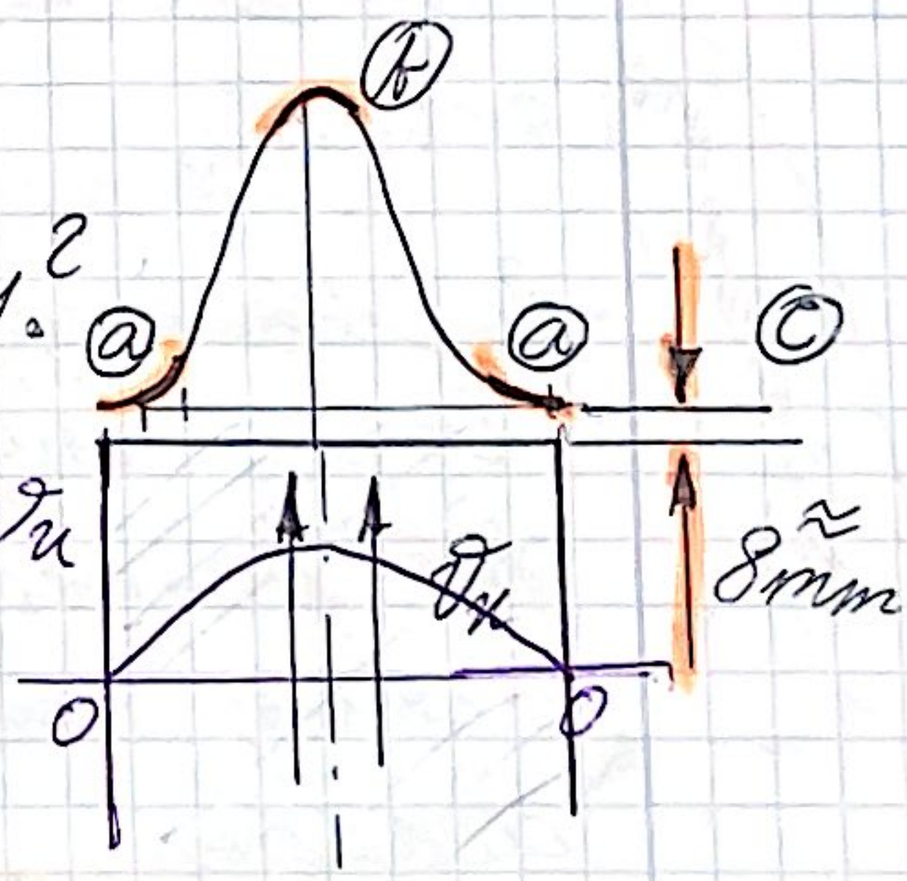
$\dot{m}_{A'} = \dot{m}_A$

$v_u S_u A' = \int S_L \cdot \vec{n} \, dA \cdot S_u$

$v_u \pi R^2 = \pi R L S_L$; $R/L = \sin\alpha$

$\boxed{S_L = v_u \sin\alpha}$

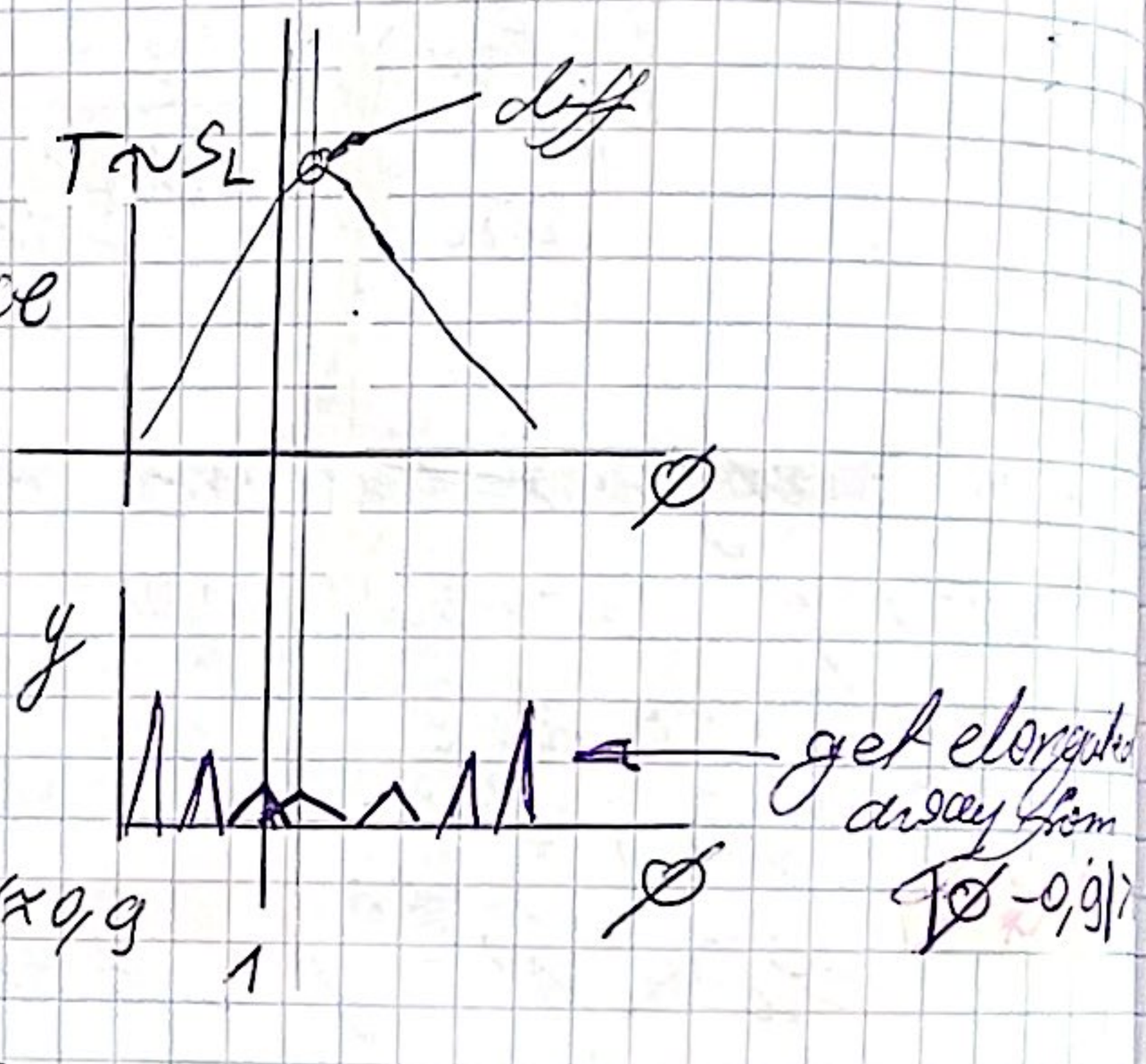
Issues : Not a perf shape. Why ?



@ viscous gas-wall interaction → parabolic profile → v_u @ wall = 0 ⇒ must increase • $\vec{n}$ component to retain flux = cst ⇒ $\alpha \nearrow$

(b) thermal diffusion: as the v_u are squeezed more and more together near the tip, it absorbs more and more heat from the burned zone thru thermal diffusion → more temp of fresh flame ⇒ S_L ↑. But $S_L = v_{u,n}$ so also v_n ↑ must; v_u ≠ const no ↑, flame becomes flatter

(c) near wall of burner, cools not adiabatic - heat losses ⇒ flame needs to heat up more before you see the front → detaches from surface



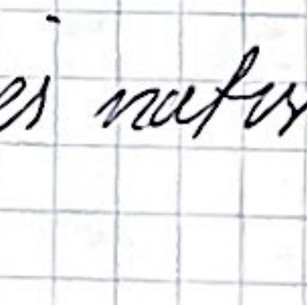
Note also: since flame slower away from $\phi \approx 0,9$ (temp lower) so α ↓ away from $\phi \approx 0,9$ so more elongated

This also comes naturally from area ratio/flux method.

or increase $\dot{m}$

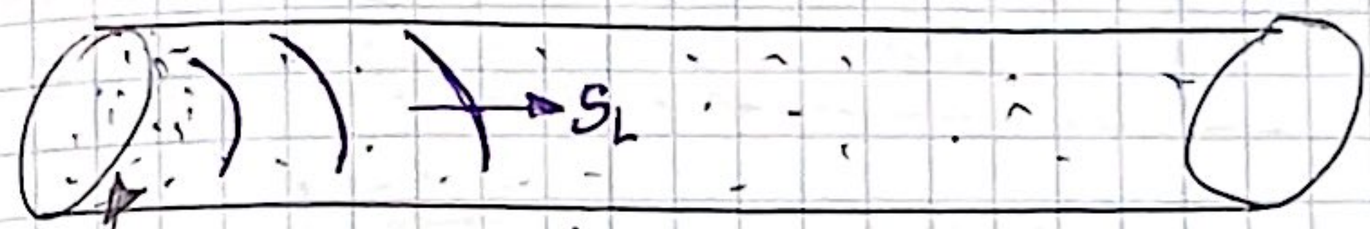
2 decreasing flame speed on flat burner only possible if it detaches from the burner — no ↑ velocity if you increase cooling, more heat losses so further detaches

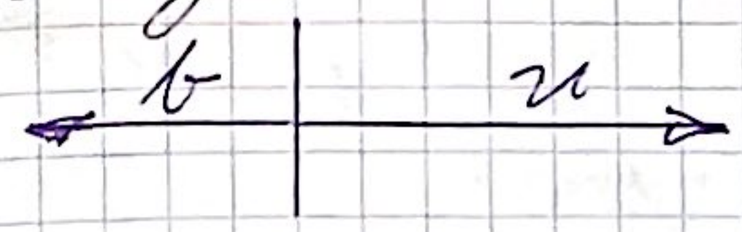
1-D assumption!



$S_L = v_n = \frac{\dot{m}}{A}$ [m³/s]

II 1 Tube method





The flame assumes parabolic shape due to:
- visc BL
- natural convection (tilted)

Simply then

$S_L = \frac{\Delta x}{\Delta t} \pm$ correction for flame tilt & curvature

or

$S_L = (V_S - V_G)\frac{A_t}{A_f}$ (WTF?)

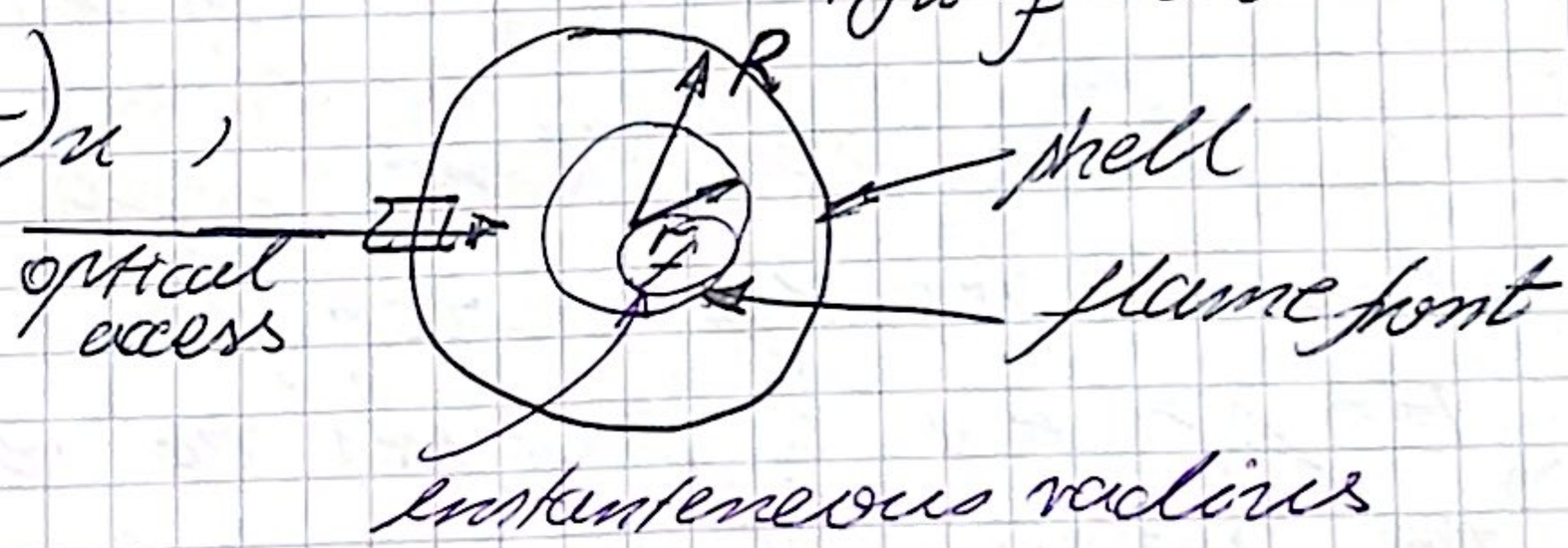
correction for "residual" velocity; correction for shape

2 Combustion bomb

- Combustible mixture ignited in center of rigid spherical vessel
- Expansion due to high T causes P&T to rise due to adiabatic compression
- $P_t \approx T_t \approx$ small for small t, esp if $R_f/R \ll$. But later ($t \gg$) $\exists$ T, P↑ causing $S_L \neq 0$. So:

$$S_L = \frac{dr_f}{dt} - \frac{1}{3}\frac{R^3 - r_f^3}{P\gamma_u r_f^2}\frac{dP}{dt}$$ pressure

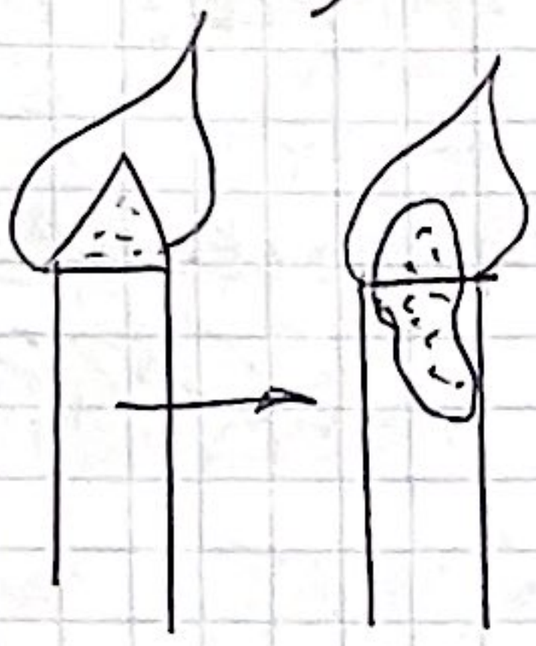
$\gamma_u = (c_p/c_v)_u$,



7. Comparison of max flame speeds

	CH_4	Ker	H_2
max $S_L[\frac{m}{s}]$	0,38	0,56	2,9
ϕ			(x10! cmp CH_4!)

8. Flame stability



$v_u \ll S_L$

FLASH-BACK

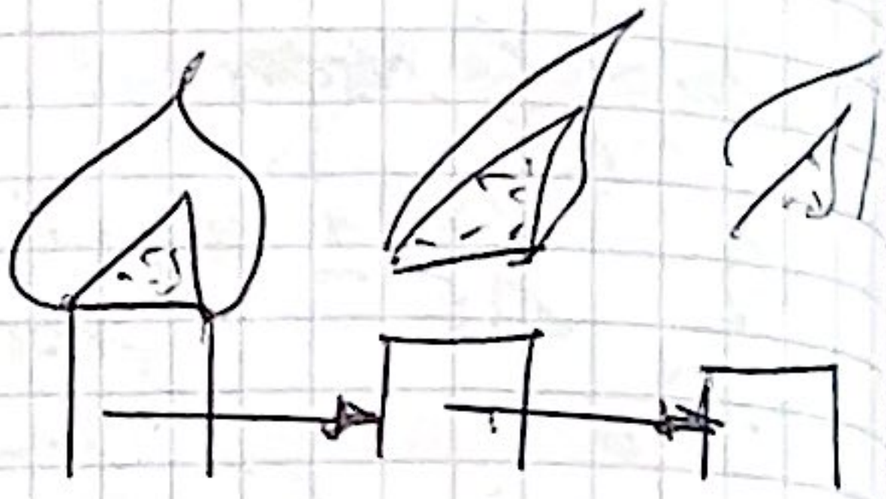
propagation back into the tube



$v_u \gtrsim S_L$

(only slightly >)

STAB



$v_u \gg S_L$

BLOW-OFF

LEAN [RICH] BLOW-OUT ≠ BLOW-OFF

→ too much air [fuel] @ T_u, so heat cannot bring T_{ad} to T_{ig} and flow extinguishes (cc not sustained)

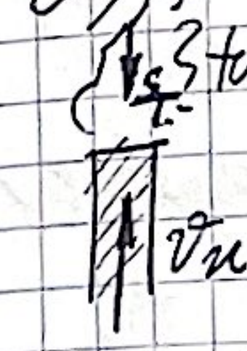
9. Flashback and its types.

FB occurs when flame propgts from a zone into the premixing section of the combustor. FB significantly increases the temp inside the premixer which is not designed for this purpose. Bonus info: FB is acc a stable phenomenon.

as flame moves back to the premix zone, it heats up the walls, so $T_{ad} = T_{flame}$ ↓ so S_L ↓ and "less FB".

a) Core ~~Flow~~ FB — only for tub — ∄ in lam.?

core FB occurs when the tub burning vel exceeds the local flow velocity in the core flow. Note that a swirler device in a typical cc may invoke core-flow FB



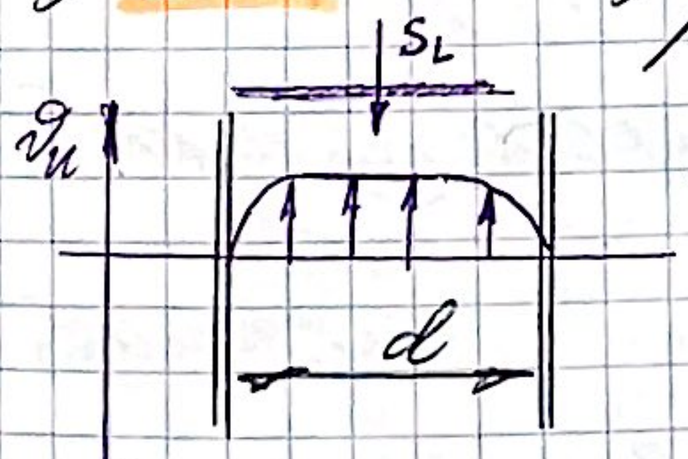
Why never happen in lam.?

Core $(S)_T \gg (S)_L$

Since tub is "unstructured", locally S_T may exceed v_n so core flow ⇐ FB.

In lam never happens cuz if S_L changes, ∝ adjusts "automatically" (+S_L too low) Tub flow doesn't have this mechanism.

b) BL FB, quenching distance



if $d \to 0$, then all throughout d vel v_n is small due to visc effects (BL), so $v_n \ll S_L$.

But $d \to 0$, heat losses ↑, also S_L reduces. (☆). The smallest d @ which the flame is not yet quenched (extinguished) is the "quenching distance".

	CH4	Ker	H_2
quench. dist [mm]	2,5	1,4	0,64

(☆) so ∃ a pt where S_L overcomes v_n near the wall @ d_q.

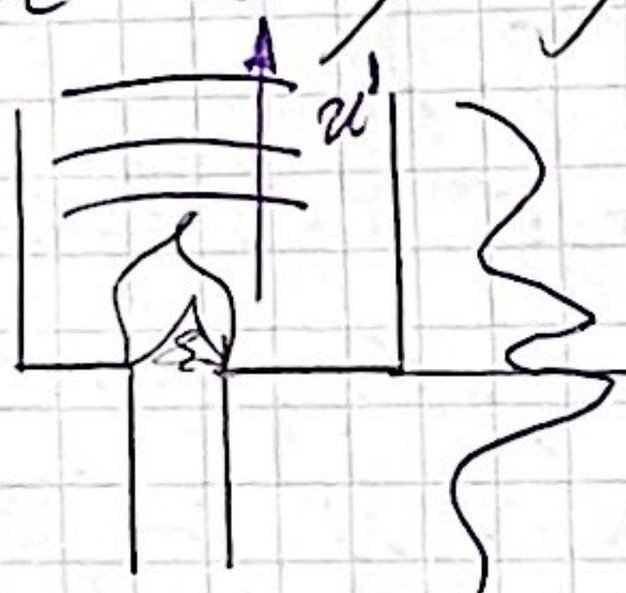
d_q is bigger (worse) in cylindrical tubes! (than // plates)

An indicator of the FB property of a mixture @ given condition is the critical velocity gradient G_F — corresponding to bulk flow velocity @ the condition of FB

$$G_F := \left.\frac{\partial u}{\partial y}\right|_{wall} \leq \frac{S_L}{\delta_q}$$

c) Thermo-acoustic generated FB

Interaction of the acoustic modes, unsteady heat release & flow structure induce large-ampl fluctuations of the flow field.



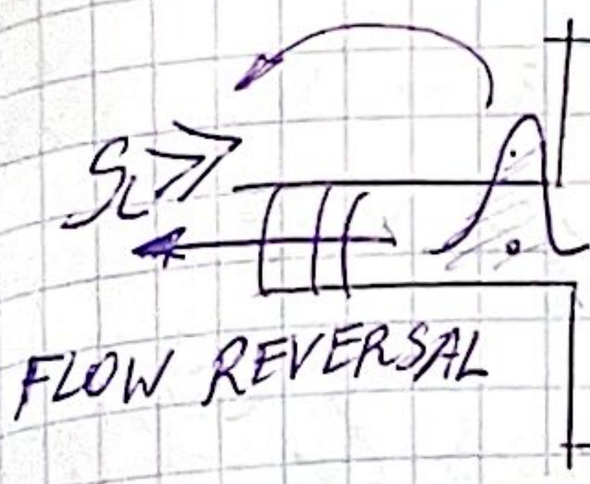
@ x_0 $u(t) = \bar{u} + u'(t)$

it may be that $\exists t = t_0$ s.t. $u(t_0) < S_L$ & flow reverses ($u' \ll 0$). Then FB. Mostly happens in turbulent. Least laminar is unable to cause such strong fluctuations.

FLOW REVERSAL

d) Autoignition FB — usually @ high P

At high P_2 (& premixed, although not limited), the mixture may spontaneously experience a temp spike & create an ignition kernel. That induces pressure fluctuations affecting velocity field & FB may occur if velocity S_L is just high enough.



high T peak = ignition kernel. may be due to sudden, strong P-Event, main flame extinguish or thrust variation, etc.

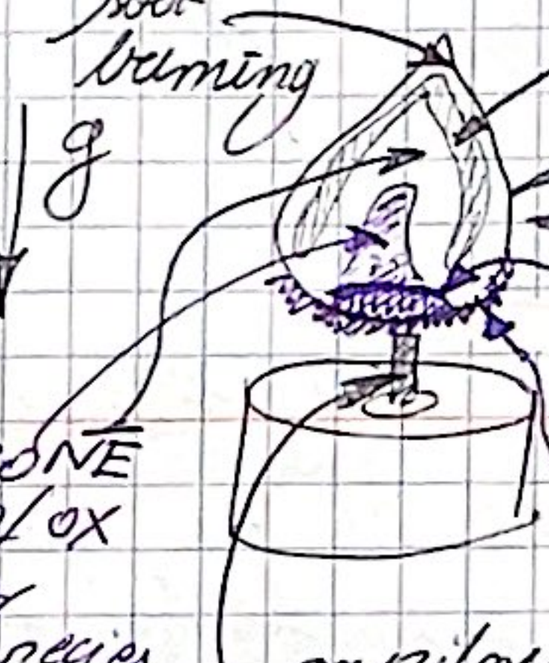
- high P destabilizes — stronger thermoac. FB
- high Φ stabilizing effect.

e) Combustion - induced vortex breakdown flashback.
∃ mainly in swirling flames (SFs). SFs induce VB — a stagnation bubble where $v_{axial} = 0$ & flow reverses. If cc is introduced, heat release interacts with vortex structures. This can move the bubble upstream causing flashback, even if the turbulent flame speed is lower than the bulk axial velocity. (if $S_L < v_{axial}$)

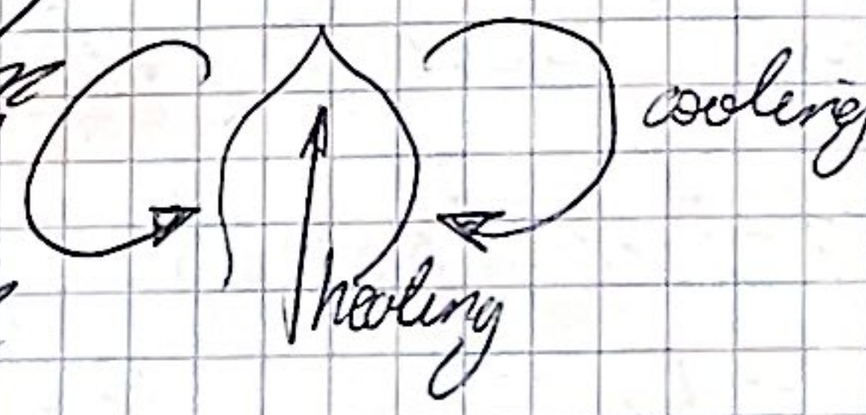
8. Diffusion flames
   - F + O are unmixed up to the flame surface
   - the transport of F + O into the rxn zone occurs primarily due to the molecular & turbulent diffusion so that they mix @ flame surface.
   - burning rate is influenced by the rate @ which F + O can reach together @ the flame surface in adequate proportions — they're diffusion limited.
   - safer (more stable)

- produce way more pollutants
- natural in the way they originate

S. Candle



- Why is flame elongated? — result of natural convection



in µ-g is spherical

- Why yellow? — incandescence of soot

Soot = conglomerated particles ~ [nm] long chains of carbon compounds.
Forms during incomplete combustion or pyrolysis ≠ UHC (molecules)

- Do hydrogen flames produce soot?

→ no?

10. Summary

DIFF	PREM
– burning @ $\phi = 1$	– burn @ ϕ = any
– FB – free	– prone to FB
– very stable ← cuz always @ right $\phi = 1$	– – " – instab ↑ ← may have too much. For 0 → may not ignite @ all.
– reliable ignition	– unreliable ignition
– broad ope envelope	– narrow ope envelope
– high NO_x, soot	– low NO_x, soot
– easier to ctrl CO	– difficult to control CO

← Flame can't propagate if FB occurs in the tube. Premix can still burn

← unless $\phi \gg 1$, then they do produce soot. But still less than diffusion

6) Experimental Combustion II – Diagnostics

1. a) CH_4 vs H_2

Which flame is more prone to FB?

– H_2 cuz S_L, $H_2 \gg$?

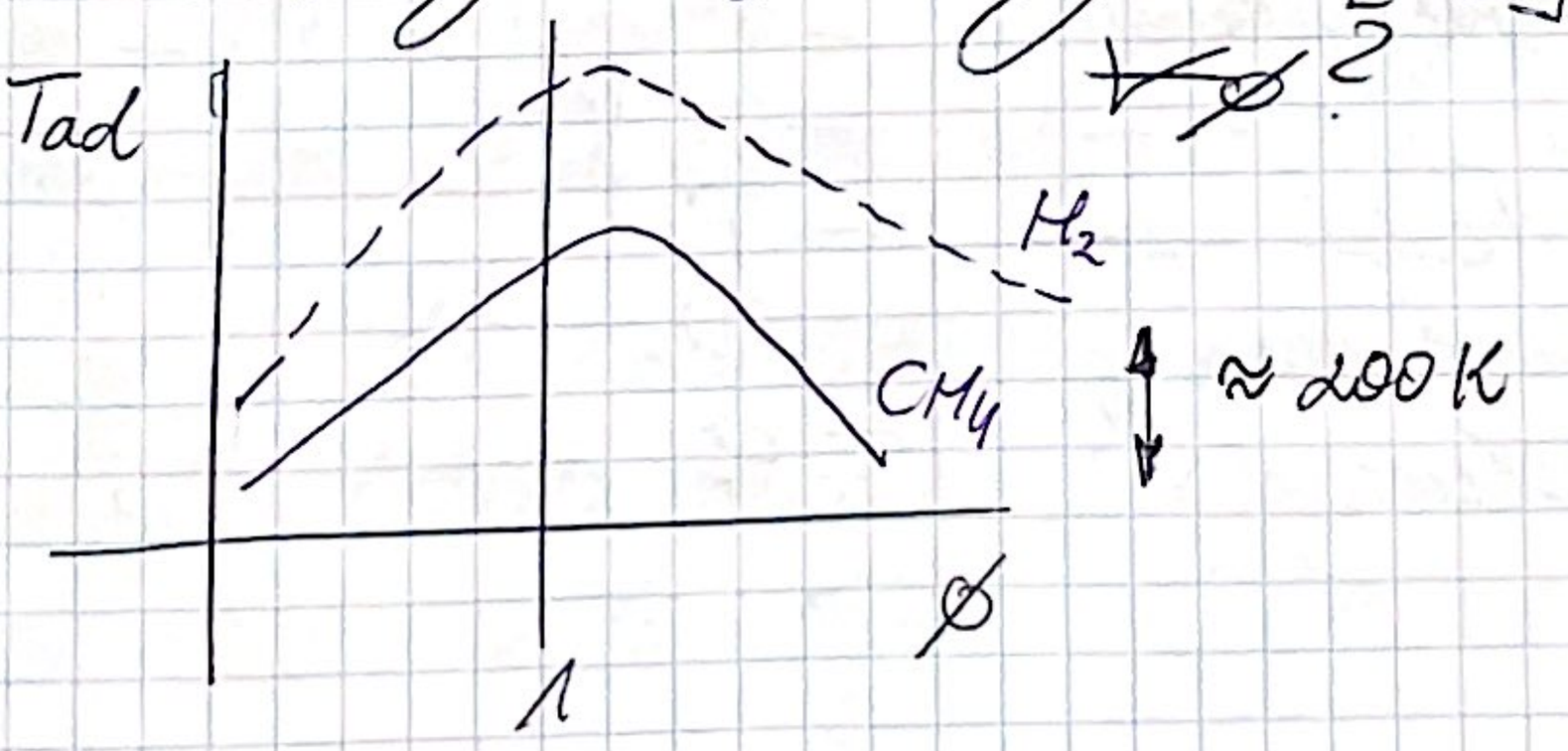
b) Do H_2 & CH_4 flames produce soot?

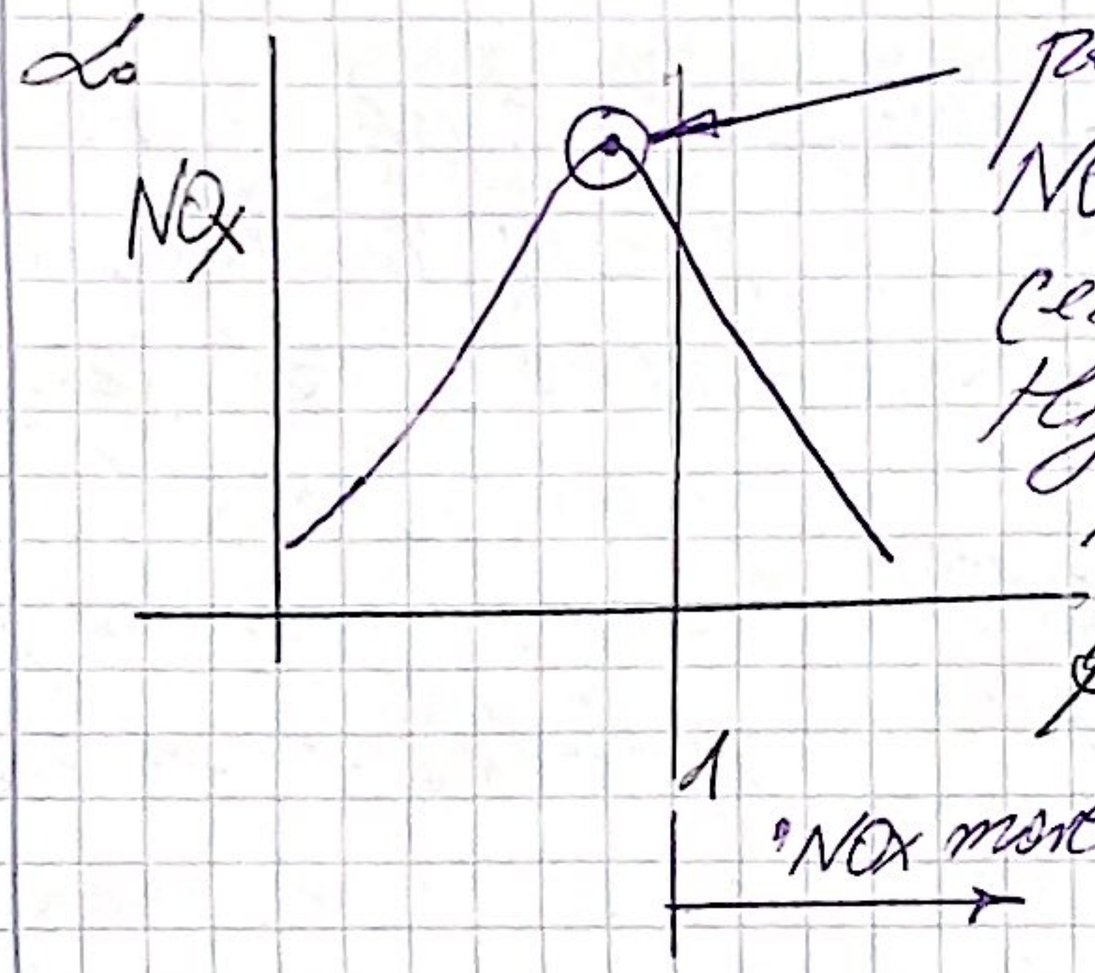
– only CH_4 cuz H_2 has no C-atoms?

c) What pollutants are most in H_2 flames than in CH_4 flames?

– NO_x cuz higher Tad ~~ϕ~~ ?

d)* → relating to c). Why $T_{ad}[H_2] > T_{ad}[CH_4]$ ~~$\forall \phi$~~ ?





peak @ $\phi < 1$. Why?
NOx needs lots of oxygen (excess) & high temp
High temp is around ϕ=1 but ox excess only if ϕ<1

NOx more acceptable @ high thrust

3. UHC = molecules
   soot = particulate agglomerated matter.

4. Measurement techniques (for your reference if you know 'em all).
   a) PIV (visualization, flow)
   b) Spray Imaging (vis, droplet size & distribution)
   c) OH-NO PLIF (vis, flame)
   d) CARS & LIGS (fs-ps diagnostics)

5. What you typically measure

CHEMISTRY	SCALAR	FLOW FIELD
- major species - transient —11— - particulate —11— - surface chemistry - pollutants	- T - X, Y - P - D - a	- mean velo - gradients (strain rate - integral scales, spectra

6. What you expect from ur measurements

1 accurate ⇒ $\varepsilon := |E[X] - \mu|$ is small
(on average, X is close to true values)

2 precise ⇒ low STD : σ_x small
with $\mu \neq \mu_{true}$ in general (doesn't have to)

3 Quantitative ⇒ know what species you're looking @

4 Non-intrusive ⇒ you don't want your measuring system to distort the true quantity.
If the scale (temp or spatial) of your measurement device is bigger than the scale of the thing you're measuring — most likely you're gonna distort the signal

5 cheap

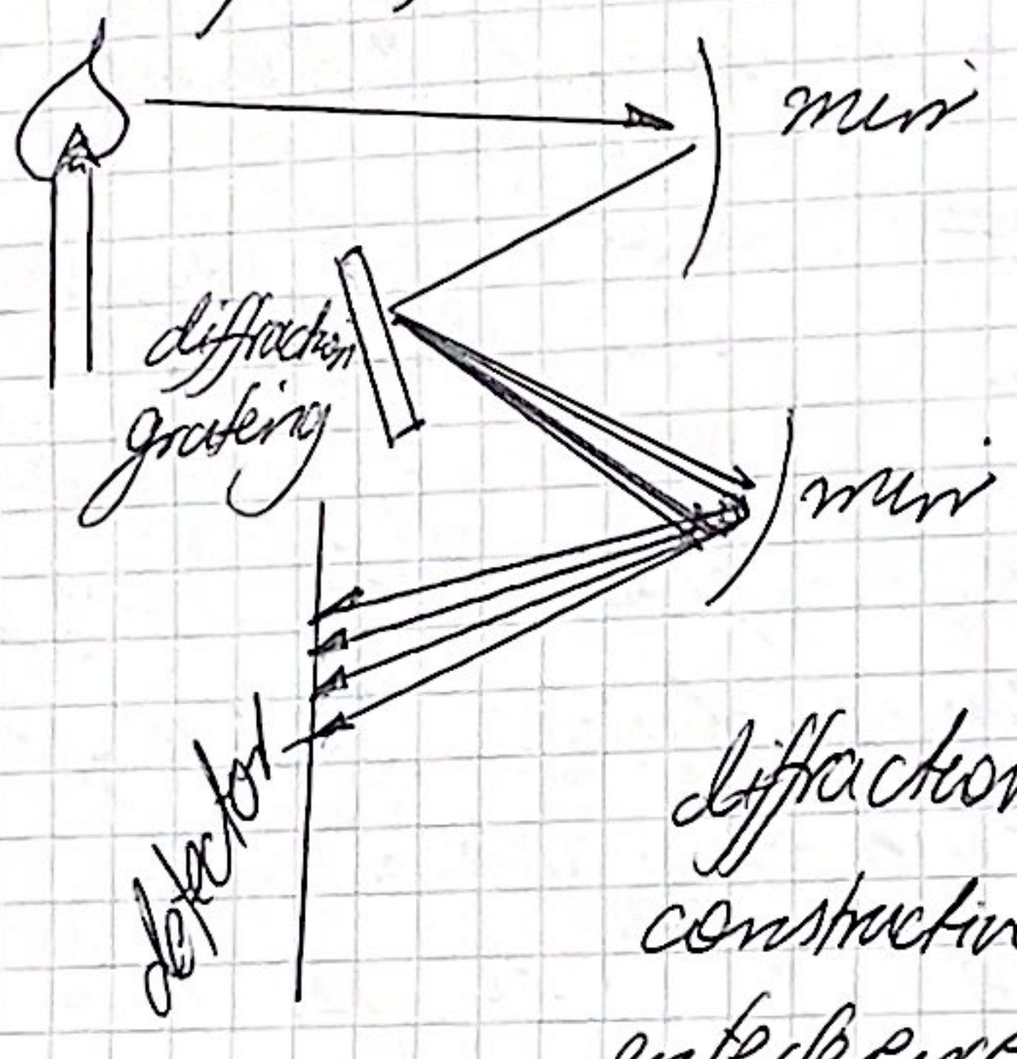
6 high T & pressure resistant

7(9) Spectrally, temp, and space resolved.
⇒ Dimensions of the probe volume and sampling rate should be smaller than the length & time scale of the phenomena we're interested in

8. Spectroscopy is the investigation and measurement of the EM spectra produced by matter interacting with or emitting EM radiation.

Spectroscopy allows for measurement of (e
— Temp
— ∅
— species (major / transient / pollut

Basic principle



Techniques using Spectroscopy:
— LIF
— CARS
— TDLAS

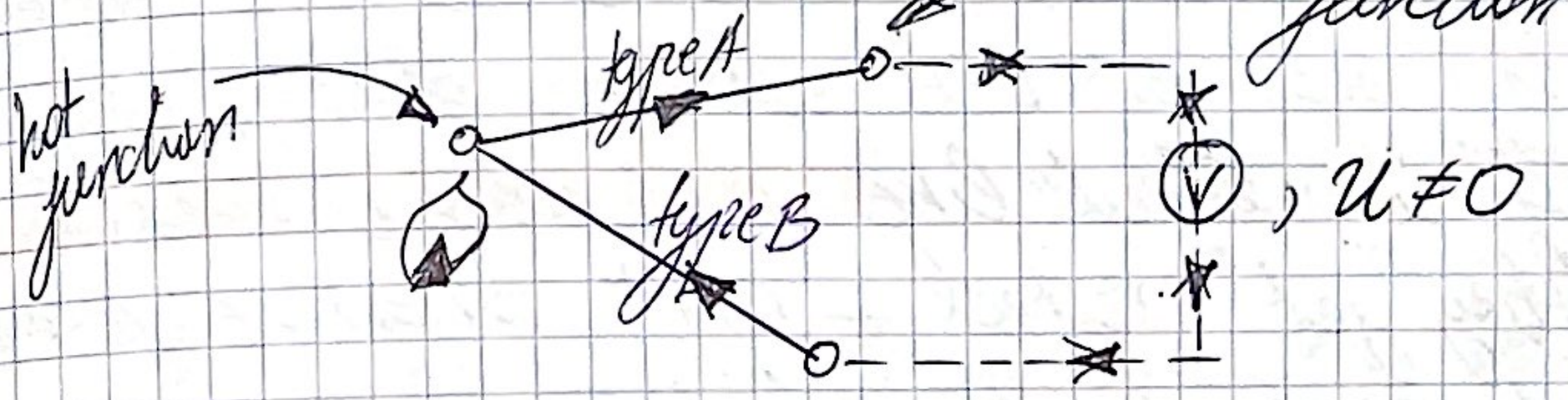
diffraction grater uses constructive & destructive interference to spatially separate polychromatic light incident on the grating

8. Family tree of cc diagnostics

9. Cel table with pos & cons (L "6", S 22)
10. Probe Measurements

a) Thermocouple TEMP

• Uses the thermoelectric effect:
∃ type A ≠ B wires & 2 hot'n cold junctions,
then ⇒ ∃ current!



when heated, electrons want to move from hot to cold. Then @ cold junction ∃ excess of e^- & @ hot junction - deficit
⇒ ∃ $\vec{U} \cong T$.

• Issues:
- Intrinsic tip
- Can melt
- Time delay / not time resolved - heating up of the tip takes time
- Radiation from the probe (losses)
- Spatial resolution limited by the probe diameter

b) Pressure Transducer / pressure gauge / manometer PRESSURE



two membrane connected into a cylinder (Bourdon tube). Uses Hook's law $F = kX$ or $M = k\theta$.

c) Exhaust gas analyzer EG composition

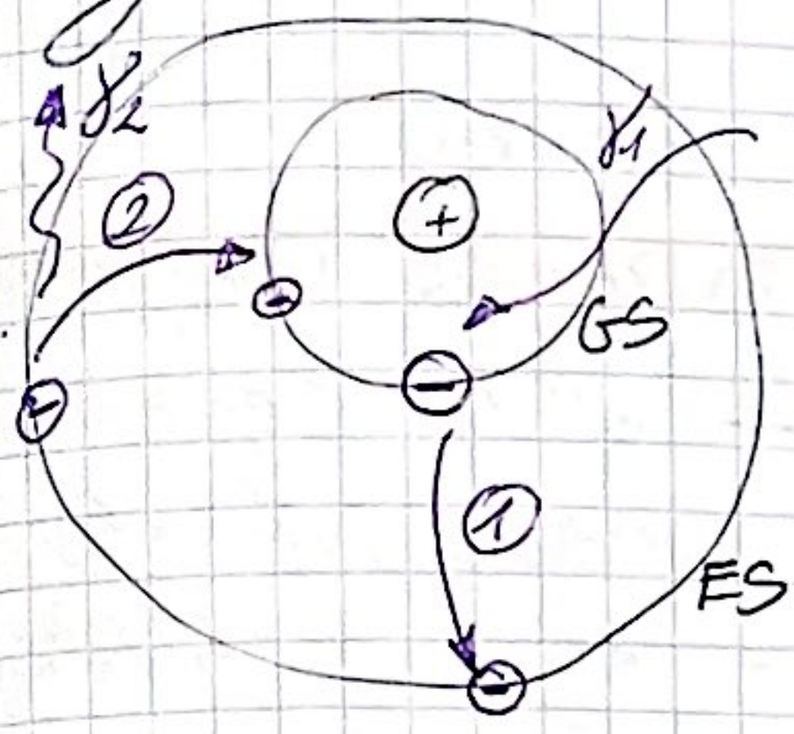
Take the EG, cool it in a tube to fix oc or ðn and analyze the "frozen" species using a variety of techniques.

11. Chemiluminescence is the natural emission of EM radiation during chem rx. Of a molecule like CH absorb heat, they get excited — CH*. When it de-excites it spont. emits radiation:

- With chem-lum you can measure:
  - ϕ in rx-zone
  - chemical process
  - heat release rate
- Cheap & non-intrusive
- ~~ϕ~~ for oral. → or diff flames
- Why soot glows yellow & premixed glow blue. Explain the differences & physical mechanisms.

PREM	DIFF
- chemiluminescence:	- incandescence
- e^- excitation & jump betw allowed en. levels	- due to temp, BB rad
- observe discrete peaks (quantized orbitals)	- cont. spectrum corresponding to a range of radiating particles
- chemically excited radicals (blue = CH*)	- soot (particulate combust.)

12. Light - matter interaction



① Incident photon γ_1 @ enough energy $E = h\nu$ causes e^- to go GS → ES. "promotion". Absorbtion (Stimulated)

② If you don't do anything, after couple seconds e^- moves ES → GS emmiting γ_2. "Spontaneous Emission"

The above explains Chemilum. Bear in mind that in chemilum. you excite with thermal energy, not a photon. But when it de-excites it does release a photon(s) as it returns to the GS. The orbits are quantized, so it emits $E = h\nu$ at a known frequency / λ. That's why you see a peak on the spectrum and not c°.

13. LASERs = Light Amplification Stimulated Emission of Radiation.

- Produces a narrow beam of light in which all of the light waves have very similar wavelengths — one specific color:
① MONOCHROMATIC. It's "organized" — polarized — has the same phase everywhere — ② COHERENT. It's very bright — ③ HIGHLY ENERGETIC & ④ DIRECTIONAL — very tight beam & concentrated.

• Pros & Cons.

PROS	CONS
— complex — expensive — cumbersome (unreliable/fragile)	— can be great resolution measurements. ϕ, HRR, species, 3D vel ... — can be used to create high speed sets for LES validation — not intrusive

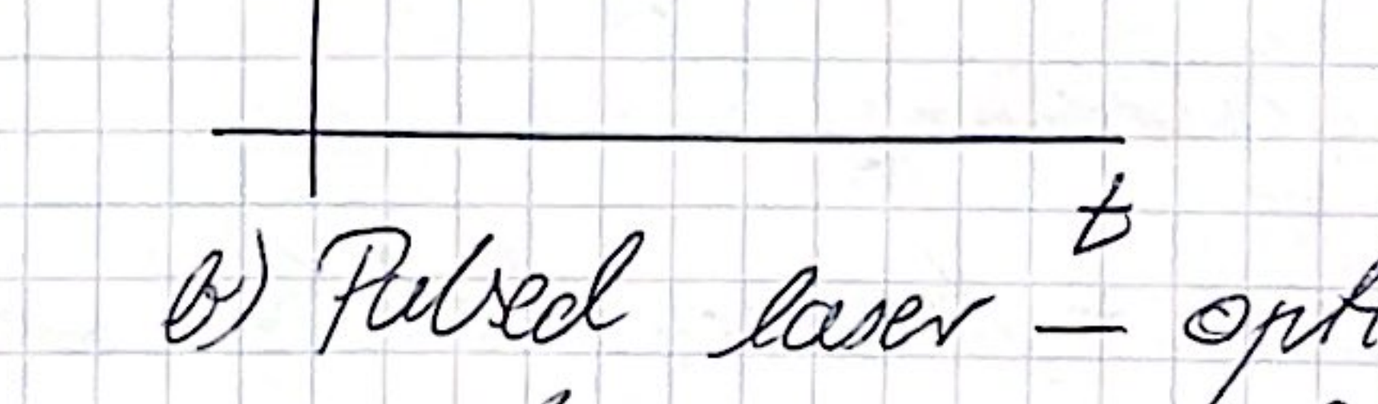
⑦ Experimental Combustion III

1. Laser Classification

a) C° — wave (CW) lasers: operate with a stable avg beam power

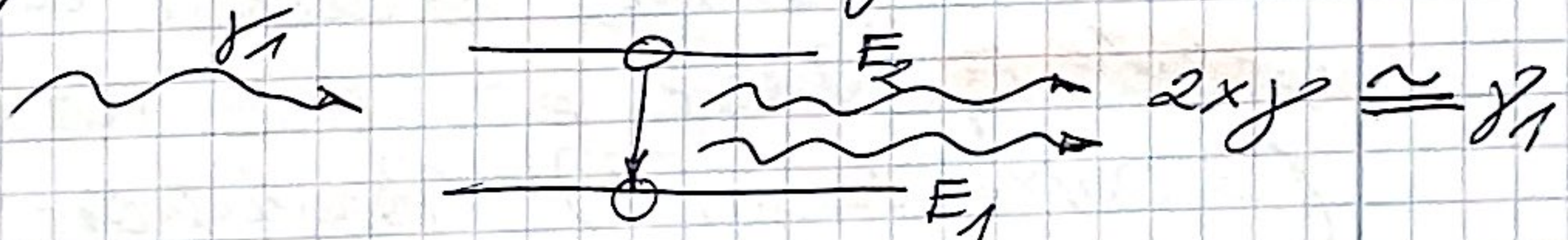


b) Pulsed laser — optical power appears in pulses of a fixed duration (e.g. 1/4 s) @ some repetition frequency. P. lasers have a higher peak power than CW



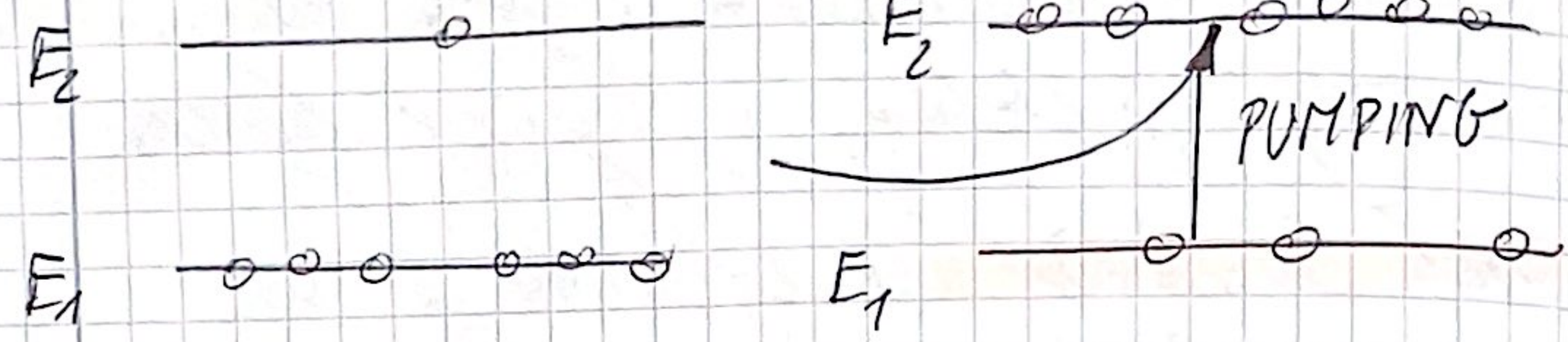
3. Class 4 lasers = 500 mW+, highly dangerous, used for cutting or etching, surgical lasers

II. Stimulated Emission. An incident photon causes an upper level electron to return to lower energy level, emitting additional "stimulated photons" whose props ≡ incidence (phase, energy, etc). This can only happen if the incidence photon is provided externally (spont emission also ∃, but for that you don't need an external photon, just e⁻ returns to GS). The amplification arises due to similarities between the incident & emitted photon. Coherent ℘ is emitted.

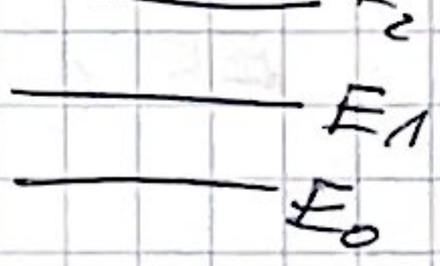


For the above to work you need to have many electrons in ES (ES energy := E_2, G_S cn := E_0).

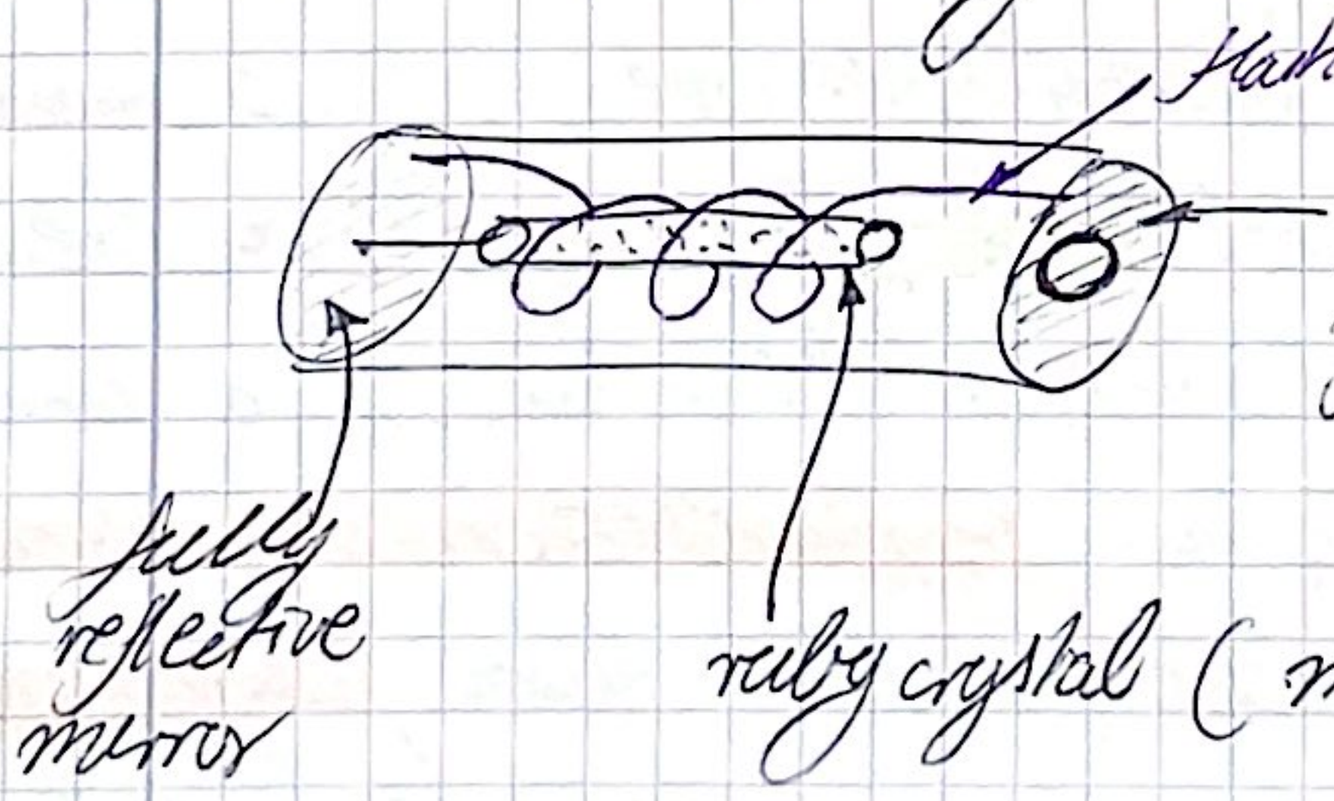
For laser action to take place you need that the stimulated emission predominate over spont emission. To do so, the e⁻ population @ E_2 needs to be more than @ E_1 (:= metastable state, see in a second). This is called population inversion. Population inversion can happen thru pumping. Once E_2 is populated, stimulated emission can take place & laser works (coherent, directional).



Problem is, excited els only stay on the ES for a short time ~10^{-8} [s], which is not long enough for them to get stm. In such conditions, population inversion cannot be sustained. To sustain it, the excited e- are required to "accumulate" @ the upper energy state till a large # of els accumulate there. This energy level which allows for sufficient exited lifetime is called a metastable state E_1. There e- live up to 10^{-3}, (10^5 times longer!). Population inversion would be impossible if not for the metastable state.



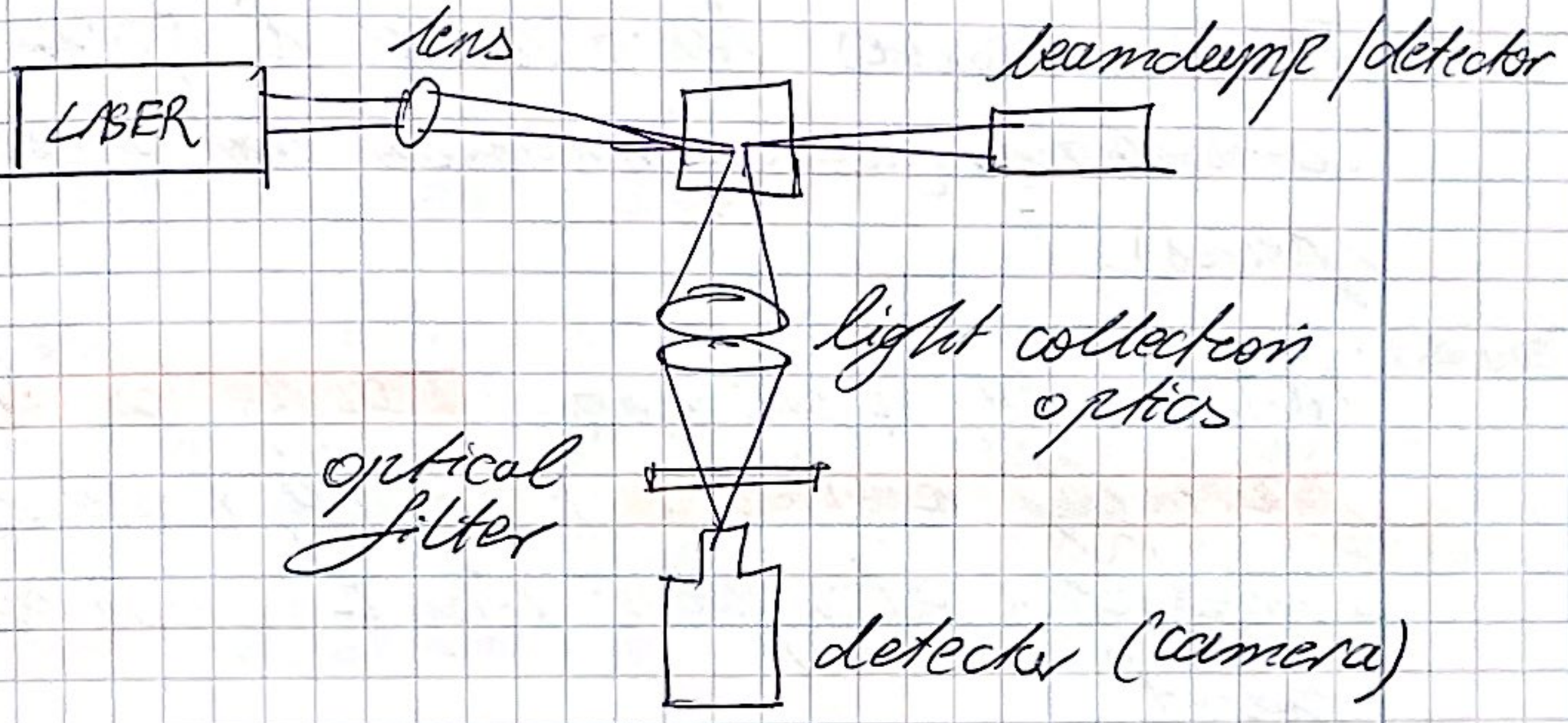
5. Laser anatomy



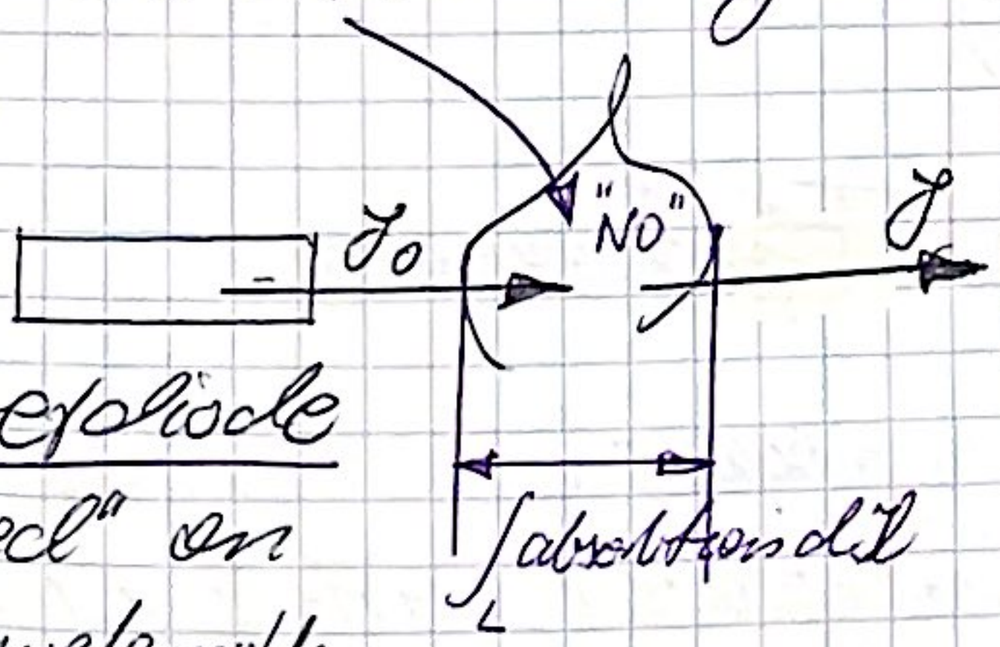
6. What happens when laser beam & gas molecule meet? — Photons can be destroyed, created or re-routed:

a) absorbtion
b) fluorescence
c) MIE scattering
d) inelastic — " — (Raman)
e) elastic scattering (Rayleigh)
f) incandescence

7. Typical laser-based diagnostic setup.



8. TDLAS — Tunable Diode Laser Absorbtion Spectroscopy. Relies on the absorbtion phenomenon. need to know exactly what λ your species absorbs.



Laserdiode
"tuned" on a wavelength absorbed by the medium

Photodiode detector:
detector that generates voltage or current when light hits it

" $I = I_0 - \int_L absorbtion\, dL$ "

Working principle: Knowing λ, you tune the laser to λ so that when it passes through species abs.

Here flame, the outgoing intensity decreases

$$\frac{I}{I_0} = \exp(-n\bar{\sigma}L) < 1$$

$\bar{\sigma}$ — absorption c-s (probability of absorption)

L — length L of medium

absorbance of a medium

$[X]$ "number density"

TDLAS measures temperature & species concentration (can approximate the amount of species).

NOTE: by construction, TDLAS is NOT spatially resolved. It can only measure integrated absorption thru L, not in point.

If 2 multiple species with same absorption length L, then need to correct for it (peak analysis.)

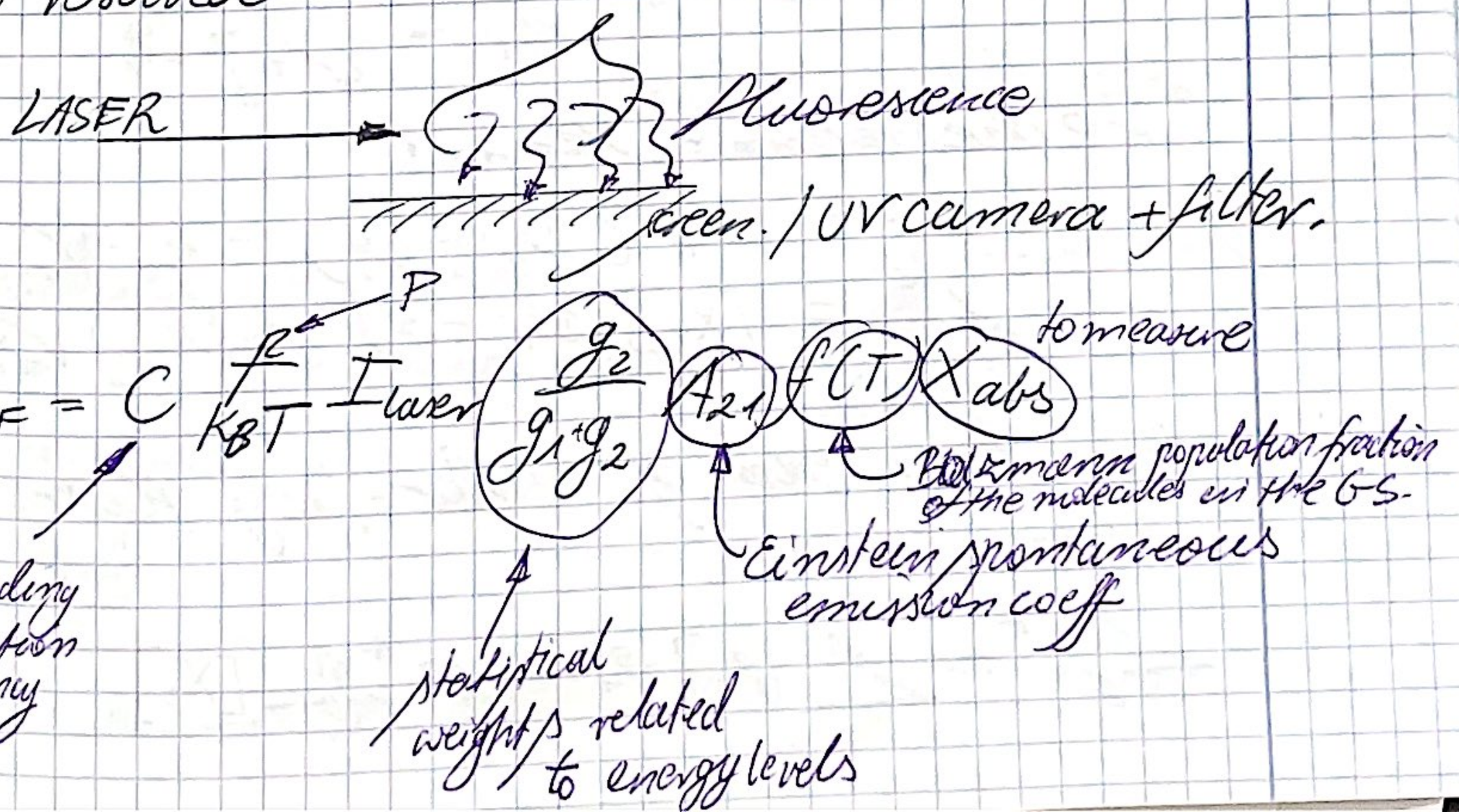
3. Laser-Induced Fluorescence

LIF is an optical spectroscopic technique where a sample is excited with a laser and the fluorescence emitted by the sample is subsequently captured by a photodetector. The flow is illuminated with a tunable laser that overlaps an

allowed electronic-vibrational-rotational transition en an atom or molecule. Molecules can relax back to GS & emit photons as the energy releases — fluorexcence. Note that usually the $e^{\ominus}$ go from the metastable state to GS so that ΔE_2 is emitted (upon collision with photon γ_1, $\Delta E_1 = E[\gamma_1]$). The excess energy $\Delta E_2 - \Delta E_1$ is used for "non-light purposes"

LIF measures concentration

Ex entance, the OH*: $\lambda_{in} = 283$ nm and $\lambda_{out} = 308$ nm. The biggest difference betw. TDLAS & LIF is that LIF (is) spatially resolved. Fluorescence is omnidirectional, not unider., so you can put a screen next to your flame & the emissions from the flame going in all dirs hit the screen so you see it resolved



⑧ Laminar and Turbulent Processes.

Pt 1. Kuo. Ch 3 — 1+2+4+11.

1. Defini the local bulk mass-avg velocty (of all species):

$$v = \frac{1}{\rho} \sum_k \rho_k v_k \text{, for } v_k \text{ velocty}$$

of k-th species. Similarly, —11— molar-avg:

$$v^* = \frac{1}{n} \sum_k x_k v_k .$$

The deviation velocty of a k-th species from the bulk is

$$V_i := v_i - v$$

$$[V_i^* := v_i - v^*]$$

} differ in magn AND! dir.

2. Define fluxes: $\dot{m}_i = \rho_i v_i$

$$\dot{n}_i = [x_i] v_i$$

So the relative fluxes:

$$J_i = \rho_i (v_i - v) = \rho_i V_i$$

$$J_i^* = [x_i](v_i - v^*) = [x_i] V_i$$

Note how sum of molar-avg fluxes is zero:

$$\sum J_i^* = \sum [x_i] v_i - v^* \sum [x_i]$$

note $[X_i] = X_i \overleftarrow{\Sigma} [X_i]$, so

$$= \left(\overleftarrow{\sum_j} [X_j]\right) \underbrace{\overleftarrow{\sum_i} X_i v_i}_{v^*} - \left(\overleftarrow{\sum_j} [X_j]\right) v^* \overbrace{\overleftarrow{\sum_i} X_i}^{1}$$

$$= [X] v^* - [X] v^* = 0. \quad (\text{MASS } ?)$$

3. Ficks Diffusion Model.

⟶ Diffusion reduces local concentrations:

$$\vec{J}_A^* \propto - \nabla X_A \quad , \text{or}$$

$$\vec{J}_A^* = -[X] \mathcal{D}_{AB} \nabla X_A \quad \text{for a BINARY MIXTURE}$$

$\mathcal{D}_{AB}$: binary mass diffusivity ("measures rate of collision between A & B)

note $\underline{\mathcal{D}_{AB} = \mathcal{D}_{BA}}$.

Then the absolute molar flux:

$$n_A = [X_A] v_A = \vec{J}_A^* + [X_A] v^*$$

$$= \underbrace{[X_A] v^*}_{\text{Molar flux of A resulting from the bulk motion of the fluid}} \underbrace{- [X] \mathcal{D}_{AB} \nabla X_A}_{\text{Relative molar flux of A resulting from species A diffusing.}}$$

Similarly:

$$\vec{J}_A = -\rho \mathcal{D}_{AB} \nabla Y_A \quad \text{and} \quad \dot{m}_A = \rho_A v - \rho \mathcal{D}_{AB} \nabla Y_A$$

4. "Reynolds analogies":

Mass, momentum & energy transport

generalized Fick "normal ρ = const"

D $\left[\frac{m^2}{s}\right]$ $J_{Ay} = -D_{AB}\frac{\partial}{\partial y}(\rho_A)$ If ρ & ρ_p = const: Fick's

$\nu = \frac{\mu}{\rho}\left[\frac{m^2}{s}\right]$ $\tau_{yx} = -\nu\frac{\partial}{\partial y}(\rho v_x)$ Newton's

$\alpha = \frac{\lambda}{c_p \rho}\left[\frac{m^2}{s}\right]$ $q_y = -\alpha\frac{\partial}{\partial y}(\rho c_p T)$ Fourier's

5. Nondim #s:

D = mass
ν = mom
α = thermal

diffusivity

- Lewis $Le = \frac{\alpha}{D} = \frac{\text{rate of energy transport}}{\text{mass}}$
- Prandtl $Pr = \frac{\nu}{\alpha} = \frac{\text{momentum}}{\text{energy}}$
- Schmidt $Sc = \frac{\nu}{D} = \frac{\text{momentum}}{\text{mass}}$

Then: $Le = \frac{Sc}{Pr}$

Often, but not always, $Le = 1$. Needa verify

MASS

MASS for a species A in a binary mixture:

$$\frac{\partial \rho_A}{\partial t} + \text{div}\, \dot{m}_A = \dot{\omega}_A$$

; recall $\dot{m}_i = \rho_i v_i$

& $\frac{\partial \rho_B}{\partial t} + \text{div}\, \dot{m}_B = \dot{\omega}_B$

$$\frac{\partial \rho}{\partial t} + \text{div}\, \rho v = 0, \text{ wk } \quad \dot{\omega}_A + \dot{\omega}_B = 0$$

& $\dot{m}_A + \dot{m}_B = \rho v$ ("total flux")

(same can be expressed in molar:

Recalling $\dot{m}_A = \rho_i v_i = J_i' + \rho_i v$

$= -\rho D_{AB} \nabla Y_A + \rho_i v$

$$\frac{\partial \rho_A}{\partial t} + \text{div}\, \rho_A v = \text{div}\, \rho D_{AB} \nabla Y_A + \dot{\omega}_A$$

and

$$\frac{\partial [X_A]}{\partial t} + \text{div}\, [X_A] v^* = \text{div}\, [X] D_{AB} \nabla X_A + \dot{\mathcal{C}}_A$$

if the "bulk, avg" vel = 0 & no source terms, then:

$$\frac{\partial [X_A]}{\partial t} = D_{AB} \nabla^2 X_A \rightarrow \text{Fick's second law of diffusion}$$

(or)

$$\frac{\partial Y_A}{\partial t} = D_{AB} \nabla^2 Y_A \quad (?)$$

This is compared to $\frac{\partial T}{\partial t} = \alpha \nabla^2 T$

For a multi component system

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div} \rho_i \vec{v}_i = \dot{\omega}_i$$

using $\vec{V}_i = \vec{v}_i - \vec{v}$ and $\rho_i = Y_i \rho$:

$$\frac{\partial}{\partial t} Y_i \rho + \nabla \cdot [\rho Y_i (\vec{V}_i + \vec{v})] = \dot{\omega}_i$$

or rewrite

$$\rho \frac{\partial Y_i}{\partial t} + Y_i \frac{\partial \rho}{\partial t} + \nabla \cdot \rho Y_i \vec{V}_i + Y_i \nabla \cdot \rho \vec{v} + \rho \vec{v} \cdot \nabla Y_i$$

using global continuity $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0$

the sum of the circled terms vanishes:

$$\rho \frac{\partial Y_i}{\partial t} + \nabla \cdot \rho Y_i \vec{V}_i + \rho \vec{v} \cdot \nabla Y_i = \dot{\omega}_i, \forall i = 1, \ldots$$

so N eqns of this kind and N unknowns Y_i. But 1 eqn can be left out cuz $Y_j = 1 - \sum_{i \neq j} Y_i$.

Pt 2. Notes from doctrine Slides

1. Can set up (4) kinds of conservation laws in CC:
   - MASS (global)
   - MASS (species), $\forall$
   - MOM
   - EN

this has to be paired with appropriate equation of state and definition of species mole.

2. From warmtz: In nature, 3 molecular transport processes ∃:

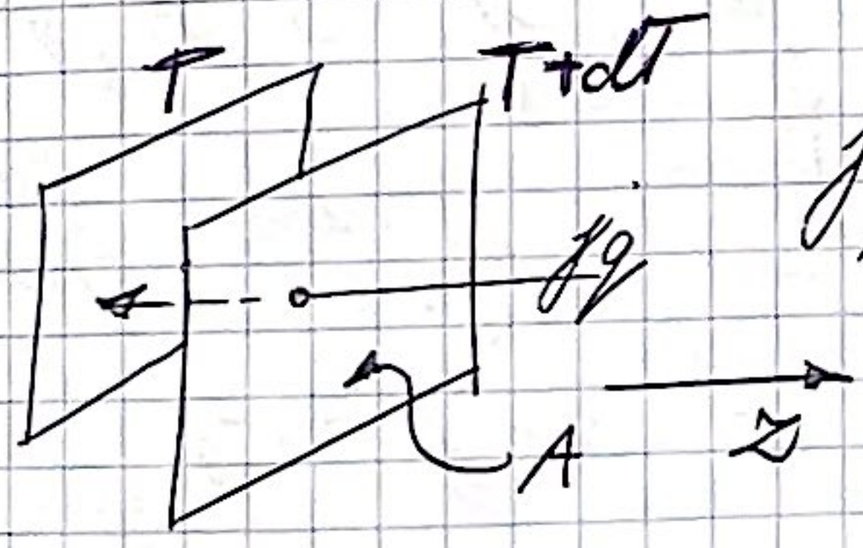
- diffusion → mas transport caused by concentration gradients
- heat conduction → en by T grad's
- viscosity → mom by vel grad's

Additionally you can distinguish other effects:

- Soret effect → mass by energy grad's
- Dufour effect → energy by concentration grad's

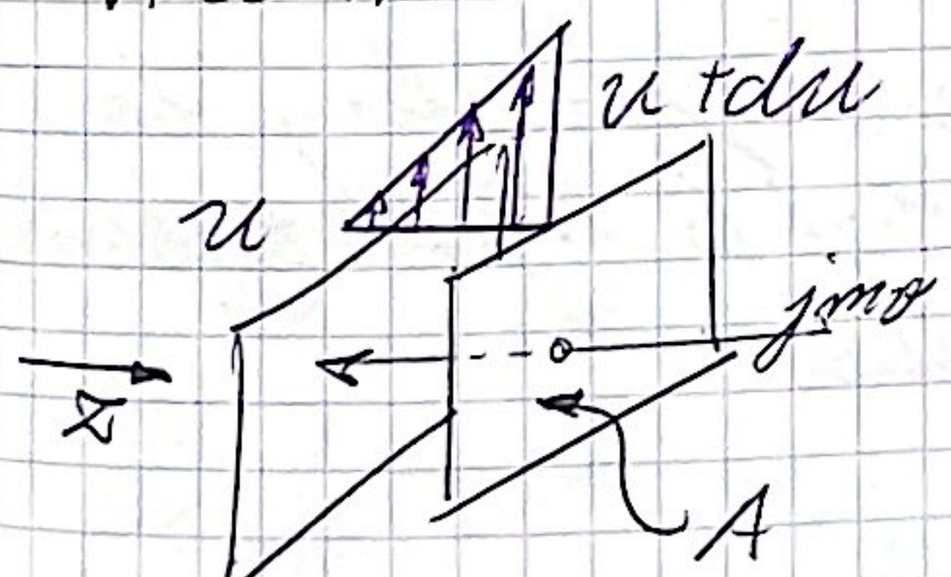
often small so neglected

HEAT CONDUCTION



$$j_q = \frac{1}{A}\frac{\partial Q}{\partial t} \overset{F.}{=} -\lambda \frac{\partial T}{\partial z}$$

VISCOSITY OF GASES



$$j_{mv} = \frac{1}{A}\frac{\partial (mv)}{\partial t} \overset{N.}{=} -\mu \frac{\partial u}{\partial z}$$

MASS DIFFUSION



$$j_m = \frac{1}{A}\frac{\partial m}{\partial t} \overset{F.}{=} -D_M \frac{\partial c}{\partial z}$$

D_M ↑ w

3. MASS from Aides

$$\frac{\partial}{\partial t}\int_V \rho\, dV = -\int_{\partial V} \rho \vec{v}\cdot\vec{n}\, d\partial V$$

→ Gauss & generalized V:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot \rho\vec{v} = 0$$

4. MOM

$$\frac{\partial}{\partial t}\rho v_j + \frac{\partial}{\partial x_i}\rho v_i v_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_j + F_{ij}$$

transient term — convection of vel with vel — pressure term — viscous term — gravity & other forces

viscous stress tensor

$$\tau_{ij} = 2\mu \hat{d}_{ij}, \text{ for } \hat{d}_{ij} = d_{ij} - \frac{1}{3} d_{kk}\delta_{ij}$$

$$d_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$$

($\hat{d}_{ij}$: deviatoric part; d_{ij}: isotropic (hydrostatic))

full stress tensor: $\sigma_{ij} = -p\delta_{ij} + \tau_{ij}$

5. Physical meaning of diffusion — the concentration of species is spreading in space with a velocity that is different from the velocity of the mixture.

6. Velocity definitions

$$v = \sum_i Y_i v_i$$

$V_i = v_i - v$ and $\sum_i Y_i V_i = 0$.

7. SPECIES' MASS:

$$\frac{\partial}{\partial t}\int_V \rho_i \, dV = -\int_{\partial V} \rho_i \vec{v}_i \cdot \vec{n} \, d\partial V + \int_V \dot{\omega}_i \, dV$$

or:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \vec{v}_i = \dot{\omega}_i$$

Define mass flux due to mass concentration gradients (Fick's):

$$j_m = \frac{1}{A}\frac{\partial m}{\partial t} \overset{"\rho v"}{=} \rho_i V_i$$ ← species deviation (diffusion)

rewriting $\vec{v}_i = V_i + \vec{v}$

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i (V_i + \vec{v}) = \dot{\omega}_i$$

$$\frac{\partial \rho_i}{\partial t} + \underbrace{\nabla \cdot \rho_i \vec{v}}_{\text{convection of mass flux with mixture bulk velocity}} = -\underbrace{\nabla \cdot \rho_i V_i}_{\text{diffusion velocity}} + \dot{\omega}_i, \text{ or}$$

$$\boxed{\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \vec{v} = -\nabla \cdot j_m + \dot{\omega}_i}$$ general i-th species MASS

8. Energy

diffusive heat flux (can be due to ∇T or ∇c) — Fourier

$$\frac{\partial}{\partial t}\int_V \rho e \, dV = -\int_{\partial V} (\rho e \vec{v} + j_q + \sigma \vec{v}) \cdot n \, d\partial V + \int_V \rho_e \, dV$$

so

$$\boxed{\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho e \vec{v} = -\nabla \cdot (j_q + \sigma \vec{v}) + S_e}$$ EN.

and $se = su + \frac{1}{2} s|v|^2 + sG$

now you can model the energy flux term

$$j_j = q_{conduction} + q_{interdiffusion} + q_{Dufour}$$

Fourier: energy flux due to ∇T:

$$q_{conduction} = -\lambda \nabla T$$

heat flux due to species diffusion: different species have diff energies which are transported with diffusion velocity V_i:

$$q_{interdiff} = s \sum_k Y_k h_k V_k$$

this is *not* convective heat transfer! convective is with bulk!

heat flux due to spec concentration often neglect

Summary:

global MASS: $\frac{\partial s}{\partial t} + \nabla \cdot sv = 0$

global MOM: $\frac{\partial sv_i}{\partial t} + \frac{\partial}{\partial x_i} sv_i v_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + sg_j$

species MASS: $\frac{\partial s_k}{\partial t} + \nabla \cdot s_k v = -\nabla \cdot s_k V_k + \dot{\omega}_k$

global EN: $\frac{\partial}{\partial t} se + \nabla \cdot sve = -\nabla \cdot (q_{cond} + q_{i-diff})$

We gotta model the $\nabla \cdot \rho_k \cdot V_k$ term. —
the mass diffusive flux term.

This term can be described exactly in case
mixture is binary: use Fick's model:

define $\dot{j}_m = \frac{1}{A} \frac{\partial m}{\partial t} = \rho_i \cdot V_i \cdot \overline{\overline{F}} - \rho D_{12} \nabla Y_i$

D_{12} = binary diffusion constant

$$\boxed{D_{12} = D_{12}(p,T) = D_{21}}$$

Then, species mass reads:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \cdot v = \nabla \cdot \rho D_{12} \nabla Y_i + \dot{\omega}_i$$

You set up $N-1$ eqns like that for $N-1$
species & Y_i is the unknown. The N-th
species concentration you retrieve from
the simplest algebraic relation: $Y_j = 1 - \sum_{i \neq j} Y_i$.
You usually leave out the most
abundant species: N_2, although not always!

$D_{H_2,j} \approx D_{i,H_2}$ is always the biggest!
Always 1 OOM > than anything else. $D_{H_2,H_2} = \max.$
$\approx 20 \cdot 10^{-5}$ [SI].

Although Fick's model works exactly for binary
mixtures, most mixtures consist of >2 species.
∃ 2 methods to deal with it:

a) "Carrier Species" method

for each of the N-1 eqns i take

$D_i = D_{iN}$, where D_{iN} is the

binary coeff of species i wrt species N.

N is usually taken as the most

abundant species. Physical meaning:

Pretend the ith species only diffuses

in the most abundant one. →

not really good! → N-th species

(most abundant) is called the

carrier species. Do not solve the N-th.

equation (D_{NN} don't!), instead

$Y_N = 1 - \sum_{i \neq N}^{N-1} Y_i$ and V_N follows

from $\sum_i^N Y_i V_i = 0$.

b) Mixture-Averaged model.

— "best thing you can have" IL.

take $D_i = D_i^M$ = composition dependent

diffusion coeff.

After Warnatz (S.25): (semi-empirical)

due to Stefan 1874:

$$D_i^M = \frac{1 - Y_i}{\sum_{j \neq i} \frac{X_j}{D_{ij}}}$$

D_{ij} ← binary

mixture-avg error is proven to be ≈10% erroneous. (at most).

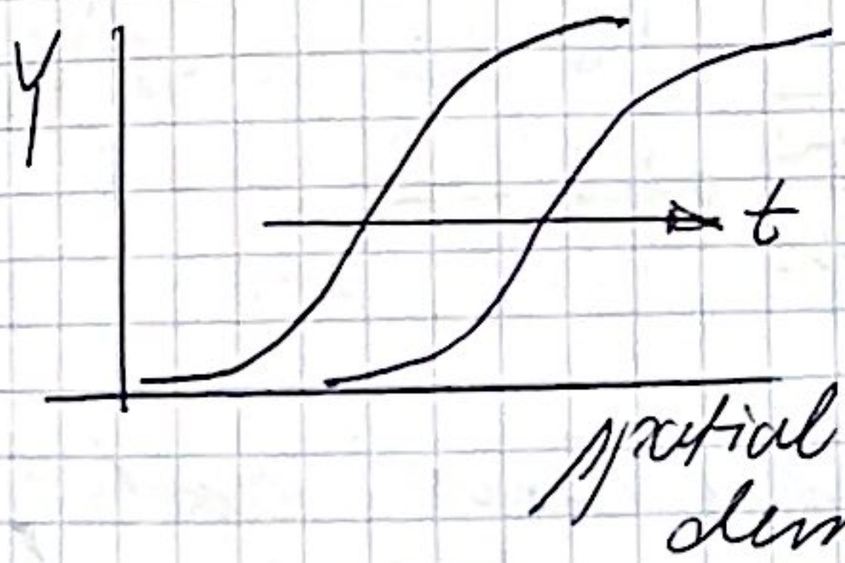
Again, leave out the most abundant species N_2, and get Y_N, V_N as

$$Y_N = 1 - \sum_{i \neq N} Y_i \quad \& \quad \sum_i Y_i V_i = 0.$$

One last look @ species MASS:

$$\underbrace{\frac{\partial}{\partial t} \rho Y_i}_{\text{transient change in mass}} + \underbrace{\nabla \cdot \rho Y_i \vec{v}}_{\text{bulk mass flux = convection}} = \underbrace{\nabla \cdot \rho D_i \nabla Y_i}_{\text{diffusion}} + \underbrace{\dot{\omega}_i}_{\text{reaction (source)}} \qquad \boxed{S_i = Y_i S}$$

Note: in SS the rates of convection = rate of diff = rate of rxn.



CONV



DIFF

$$d \approx \sqrt{D(t - t_0)}$$

9. Due to the definition of Lewis #:

$$Le = \frac{\alpha}{D} = \frac{\alpha}{D_i^M}$$ ← avg-mixed diff coeff.

it is true that $Le \approx 1$ for almost all basic species (N_2, CO, OH, O_2, CH_4) ... BUT H & H_2! So often it is set $D_i^M = Le\alpha \approx \alpha$, $\forall i \neq H_2, H$. H_2 & H have very small

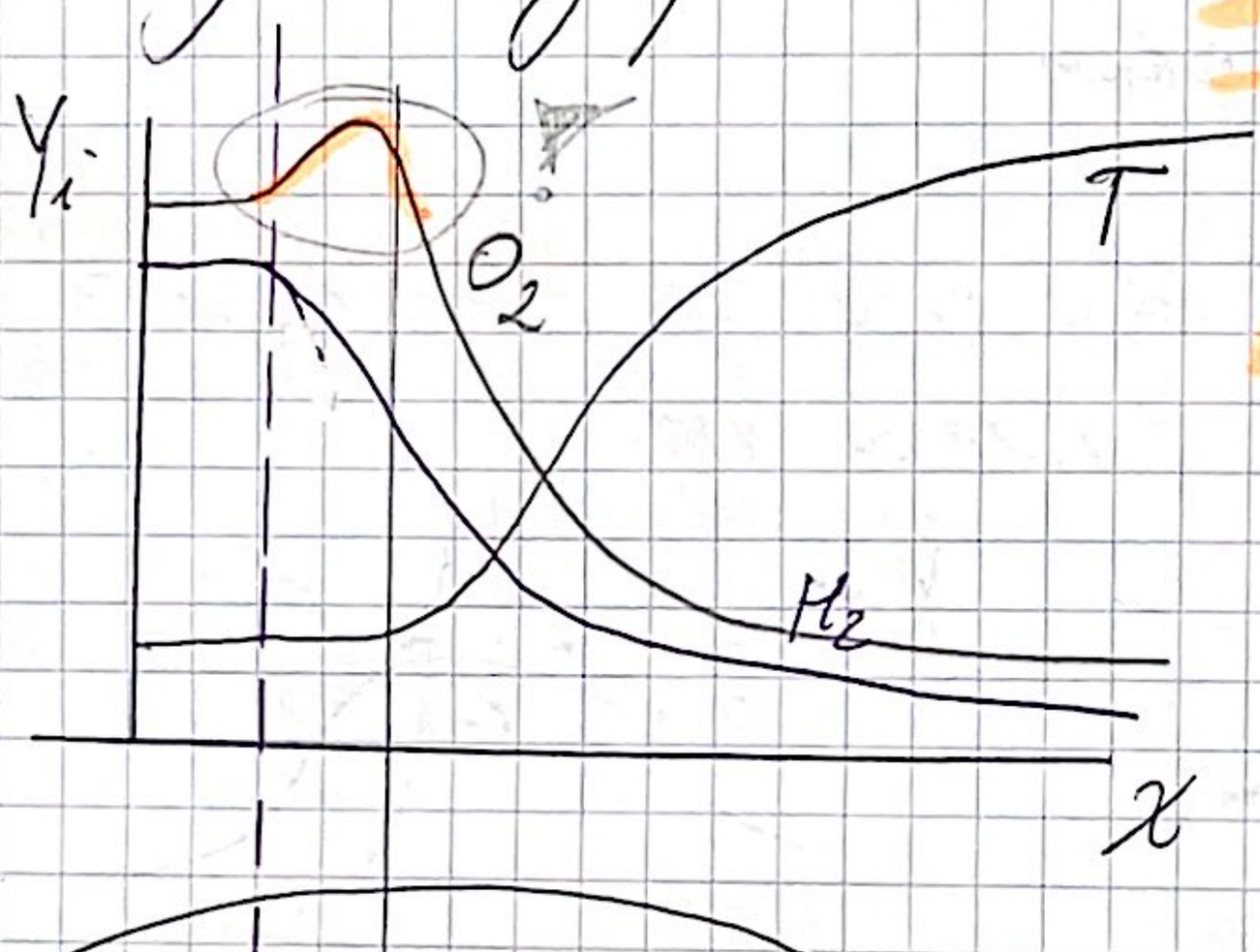
NOTE: Mixture-averaged transport is the transport of the substance of interest through a medium!

cuz $W \leftarrow !$ { always: $Le_{H_2} = 0,3$ } means
$Le_H = 0,18$ } mass diffusion
is much greater than heat diffusion! ★

In general, though, $Le := \frac{\alpha}{D} = \frac{1}{D} \frac{\lambda}{\rho c_p}$

or $D = \frac{1}{Le} \frac{\lambda}{\rho c_p}$, so D = function of species Lewis, mixture th. conductivity mix. ρ, mix. sp. heat.

10. the famous graph: → Exam Question!



H_2 diffuses faster than heat (Temp) and faster than oxygen (differential diffusion: $Le\, H_2 = 0,3 < Le\, O_2 = 0,7$), so hydrogen concentration reduces earlier (cc consumption or diffusion to product zone or both?) So to keep $\sum Y_i = 1$, O_2 must locally increase (local maximum) before it starts getting consumed in the combustion zone.

DIFFERENTIAL DIFFUSION = strong difference between α & D_i of a species, i.e. if $|Le_K - 1| \gg$.

Always: $Le_{H_2} = 0,3$ } means
$Le_H = 0,18$ } mass diffusion
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In general, though, $Le := \frac{\alpha}{D} = \frac{1}{D} \frac{\lambda}{\rho c_p}$

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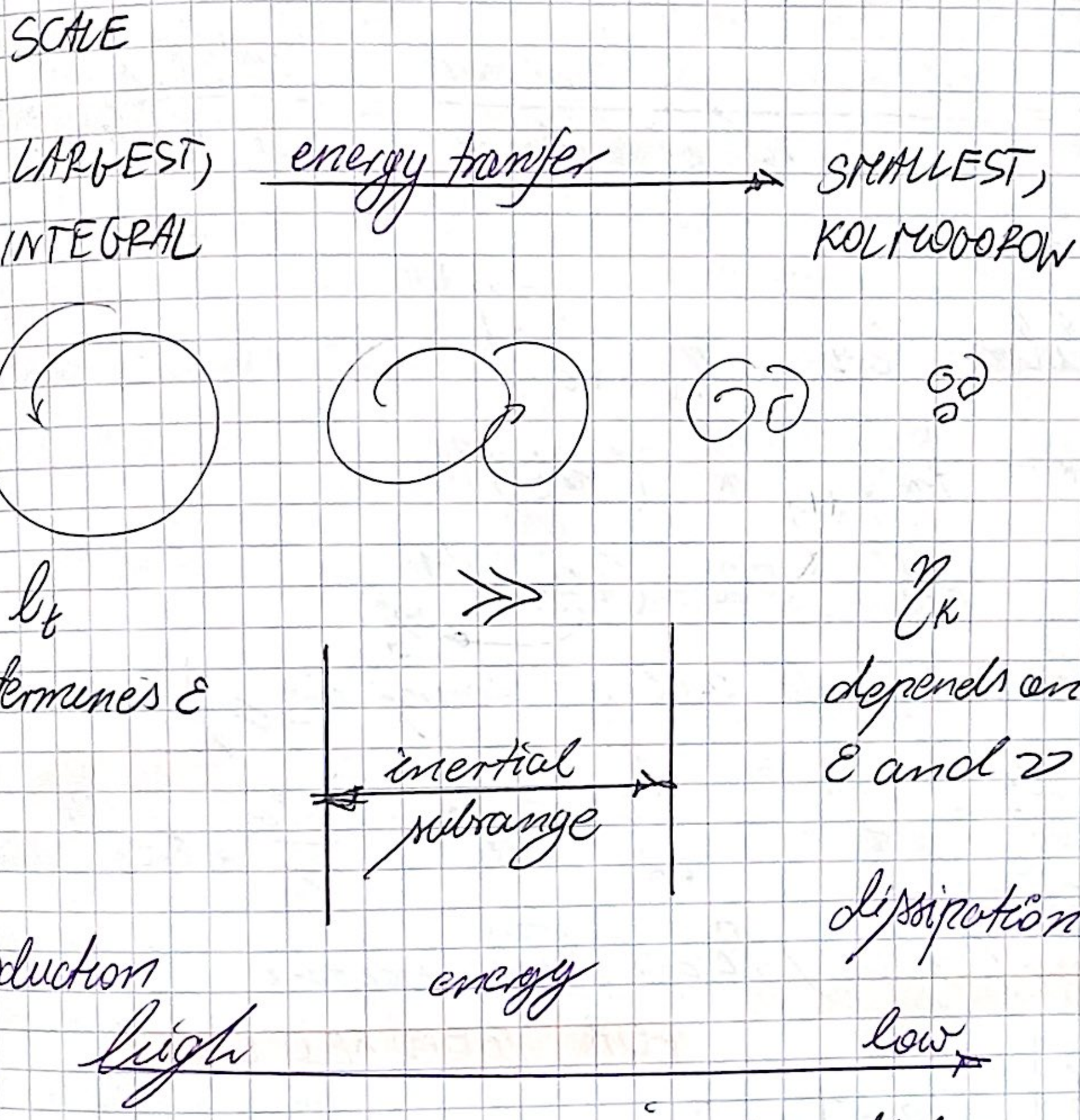
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11. Phenomenological description of turbulence

Turbulence is a connection of eddies of different sizes- Energy is cascaded from large to small scales and is dissipated @ the smallest scales @ rate $\varepsilon \left[\frac{m^2}{s^3}\right]$



Energy transfer rate from integral to Kolmog. scales $\Leftrightarrow \varepsilon$ = dissip. rate — en. cost is small eddies

In EN, this dissipation is denoted as χ_{diss}. Though small comp to heat release rate, it's important because affects the smallest eddies that can disturb the flame front and thus alter cc-rate.

∃ a rule of thumb below $Re_{tb} \equiv Re_t$

u' @ l_t → RMS velocity of large scale fluctuations $u'(l_t)$; $l_t \equiv$ integral scale.

$$Re_t = \frac{u'(l_t) \cdot l_t}{\nu}$$

And estimate for ε:

$$\varepsilon = \frac{\text{tot kin. en. per unit mass}}{\text{time needed for diss. ep.}} = \frac{u'^2(l_t)}{u'(l_t)^{-1} \cdot l_t} = \frac{u'^3(l_t)}{l_t}$$

12.

Kolm len $\eta_K = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$

— " time $t_K = (\nu/\varepsilon)^{1/2}$ m/s

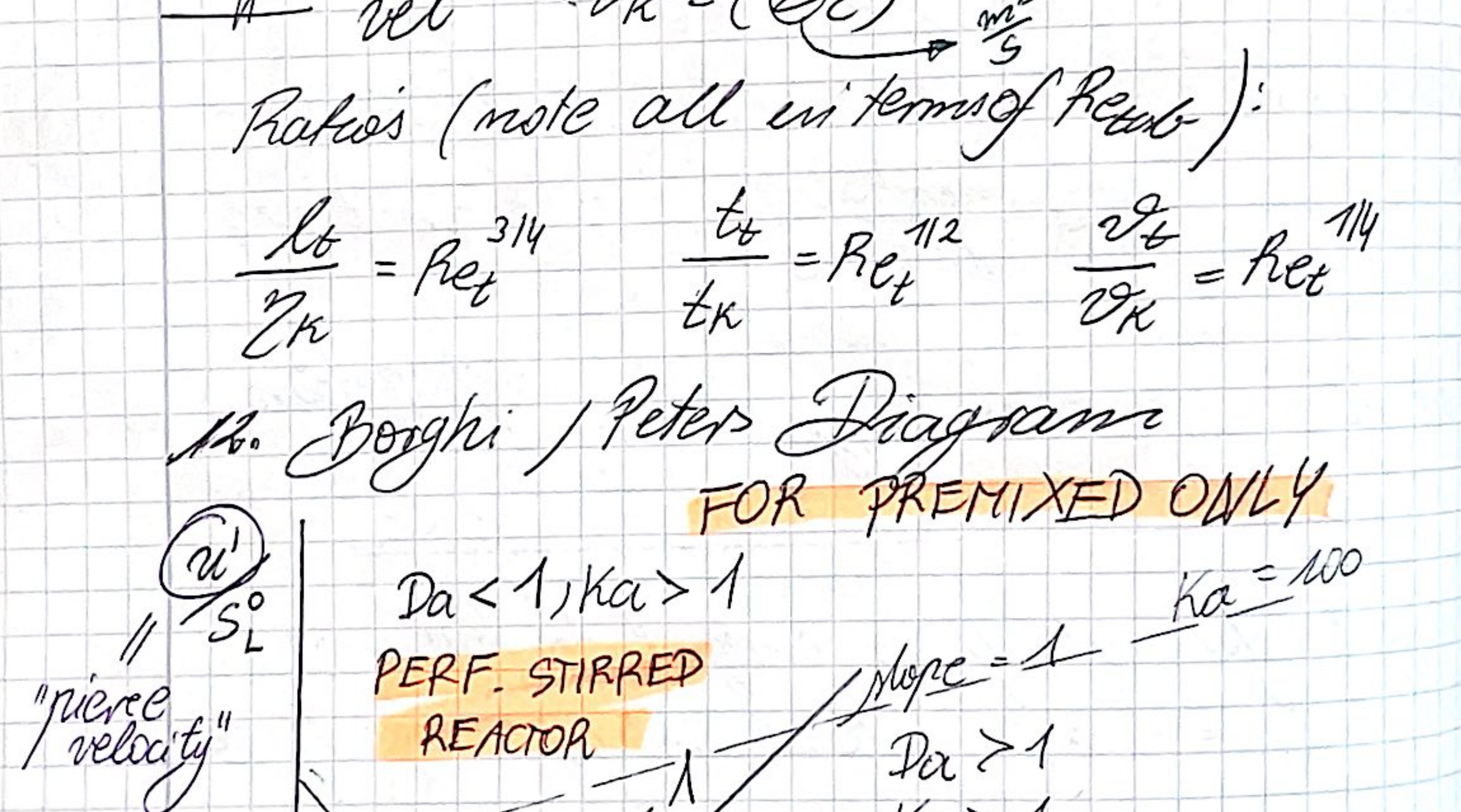
— " vel $v_K = (\nu\varepsilon)^{1/4}$ ← $\frac{m^2}{s}$

Ratios (note all in terms of Re_{tb}):

$$\frac{l_t}{\eta_K} = Re_t^{3/4} \qquad \frac{t_t}{t_K} = Re_t^{1/2} \qquad \frac{v_t}{v_K} = Re_t^{1/4}$$

13. Borghi / Peters Diagram

FOR PREMIXED ONLY



... of an isobaric process

u' = RMS velocity fluctuations of the oncoming turbulence

l_t = biggest integral turbulence length scale

δ_L = laminar unstretched flame thickness (flat)

Define chemical time — time needed for a freely propagating, flat flame to propagate its own thickness

$$t_{chem} = \frac{\delta_L}{S_L^0}$$ (interpretation: small t_{chem} means S_L^0 is v-fast, so resistant to oncoming disturbances)

Define Damkhöler # = ratio of the macroscopic time scales (integral) and chemical time:

$$Da = \frac{t_t}{t_{chem}} = \frac{l_t}{u'} \Big/ \frac{\delta_L}{S_L^0} = \frac{l_t S_L^0}{u' \delta_L} = \left(\frac{l_t}{\delta_L}\right) \Big/ \left(\frac{u'}{S_{L0}}\right) = \frac{"x"}{y}$$

If $Da < 1$, then t_{chem} ↑, so flame slow, not "resiliant" enough, meaning all oncoming turbulence u' will "mix" the flame front, will tear it apart — perfectly stirred reactor. No such thing as "flame front"

Now define the Kalovitz # = ratio of the chemical time to Kolmogorov time:

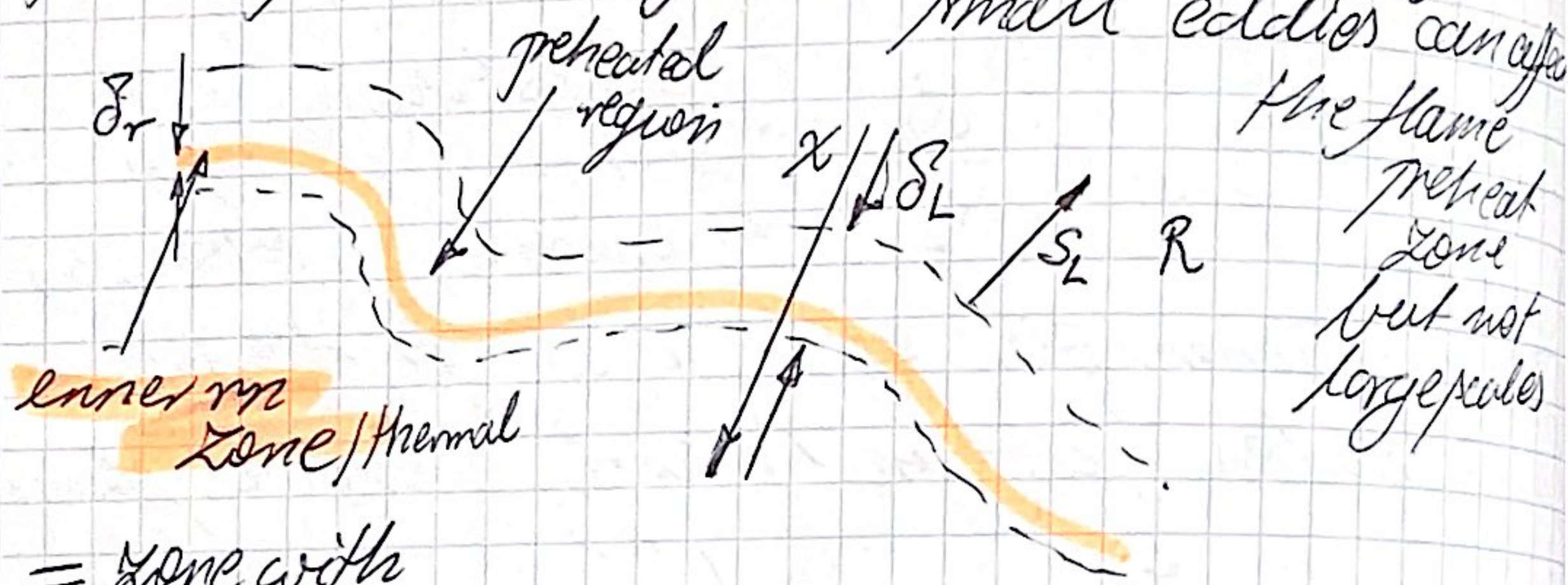
$$Ka = \frac{t_{chem}}{t_K} = \frac{\delta_L}{S_L^0} \Big/ \frac{\eta_K}{u'} = \left(\frac{u'}{S_L^0}\right)^{3/2} \left(\frac{l_t}{\delta_L}\right)^{-\frac{1}{2}} = \frac{y^{3/2}}{x^{1/2}}$$

$$Ka = 1 \Rightarrow x = y^3$$

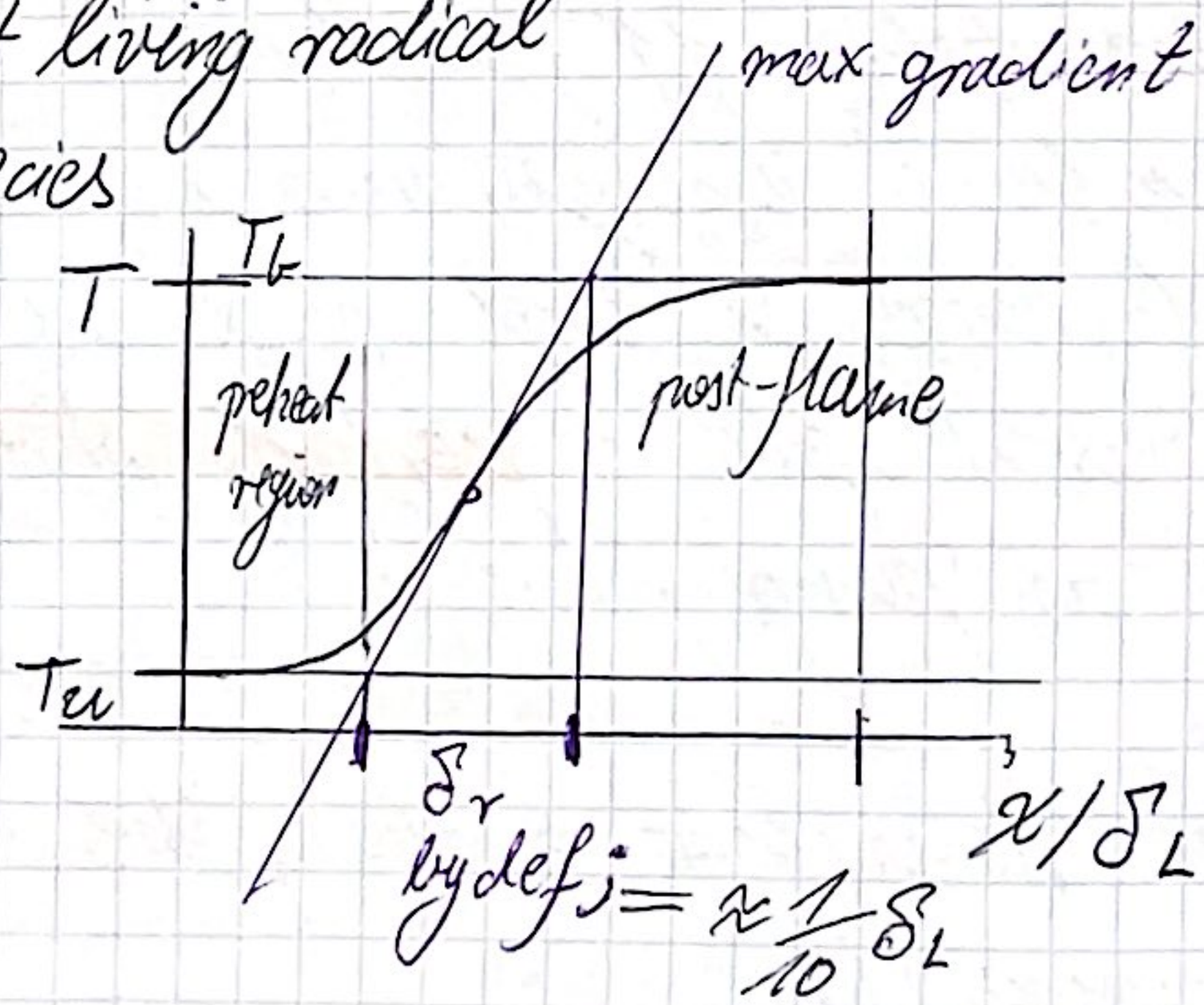
Chatty G explanation:

"Turning Points":

1) $Ka = 1 \rightarrow$ the tiny Kolmogorov eddies become quick enough to poke through the flame front – they disturb the preheat layer



= zone with intense heat release, sharp temp grad & short living radical species



2) For methane-air mixture, the rx zone is so thin that the stamp $Ka = 100$ marks an additional point where, if u' large enough and l_t small enough, the eddies can change the reaction zone

not only preheat zone.

3) $Da = 1 \rightarrow$ all eddies can affect the flame preheat zone

Now the regions:

A) Laminar corner:

- the flow is quicker than the flame is fast, and every eddy is smaller than the flame is thick, you see a razor-thin, almost perfectly flat sheet of burning gas

B) Wrinkled flamelets: $u'/S_L < 1$

- the eddies are large but slow — they fold the sheet, expanding its area. Chemistry easily outruns the effect of folding, so each wrinkle is internally homomorphic to a laminar flame. (Crepê paper wrinkles)
- the smallest eddies are too slow to alter the flame structure ($Ka < 1$)

C) Corrugated / torn flamelets:

- Big eddies are now faster than before (faster than the flame, $u'/S_L^0 > 1$). Folds steepen into cliffs, sometimes tearing & forming islands. But the inner structure of the flame front / flamelet survives because even the smallest eddies are too slow ($Ka < 1$).

D) Thin rn zone:

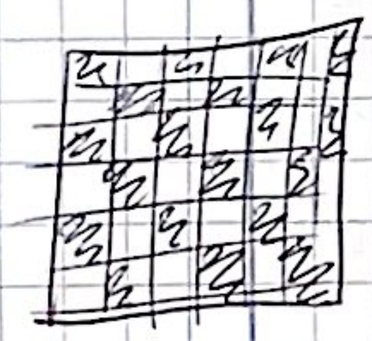
modified preheat/rn zone
for flamelet



— Crossing the Ka line is like opening the gate for Kolmogorov (smallest eddies). They shred the preheat layer, thickening the flame a little (many island, flame front preheat region, and in severe cases Ka >> 100 — rn zone) severly disturbed), but chemistry is still faster than the fluid-enhanced changes (eddies external influence) — Da > 1. Under a microscope you'd see a fuzzy halo with a sharp, luminous core

but only indirectly - thru the preheat region

E) PERfectly stirred reactor. = Da < 1



— External eddy fluid mixing owns over too small chemical time. By the time any parcel could finish reacting, new turbulence has ripped it apart and remixed it. What remains is not a flame front at all — just a hot, statistically perfectly mixed reactor.

all eddies can now disturb the reaction zone directly

Revesion of what Da, Ka, u'/S_L^0 acctuallf mean for guick edentification:

	< 1	> 1
Da/S_L^0	will never penetrate the flamelet ($u' - S_L^0 < 0$), will never tear it, or make islands.	all eddies (big or small) can now penetrate the flame ($u' > S_L^0$). This does not say anything if the internal structure is changed or not (depends on eddy size, Ka).
Ka	Small eddies too big to change the internal structure of the flamelet. Flame front still homomorphic to laminar front.	Small eddies are small and energetic enough (fast) to change the internal structure of the flamelet. This usually means changing the preheat region only, but in severe cases, Ka > 100, these eddies can also change the reaction zone!
Da*	Reaction time is so slow, by the time anything reacts, everything will get re-mixed, new turbulence will have ripped the flame front apart. The notion of flame front no longer exists, only perf. stirred reactor.	Time needed for them is still faster than the external fluid influence of the eddies. The flame front still exists, though might be severely torn, corrugated, non-homomorphic to laminar one anymore.

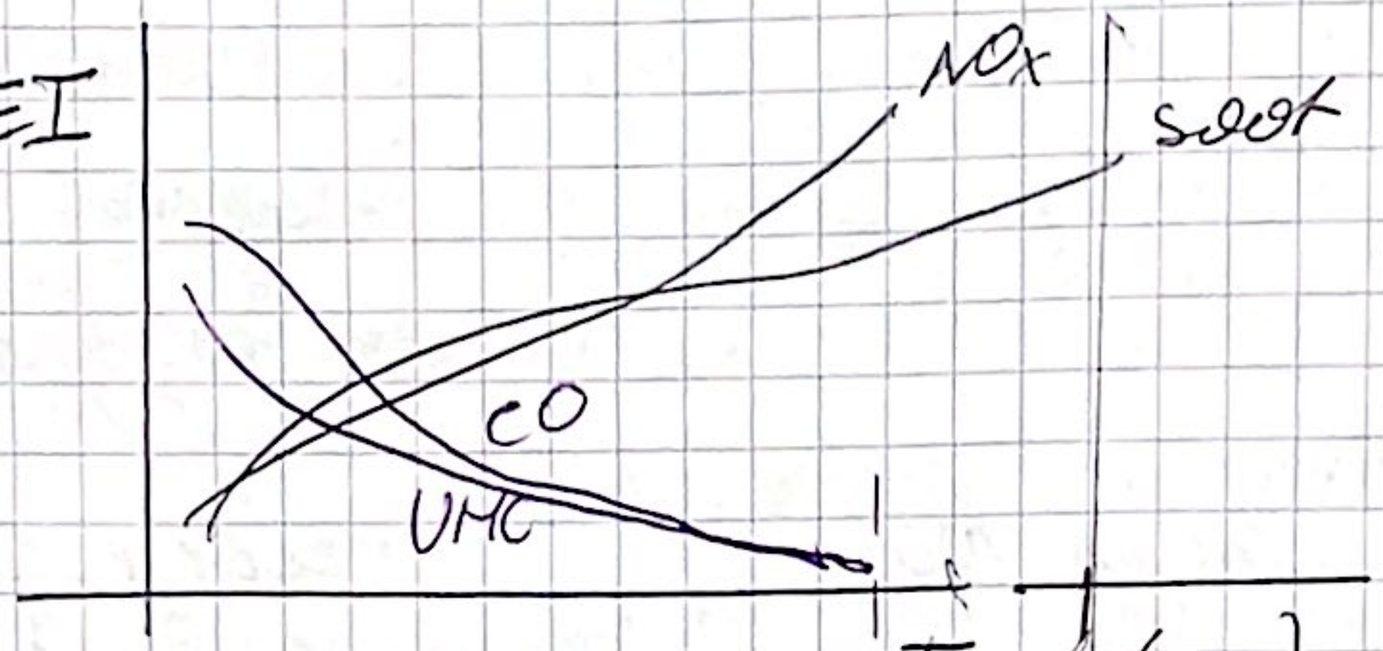
* = note how the quotient "> 1" denotes that the flamelet "opens for new modifications", while Da has it for "< 1".

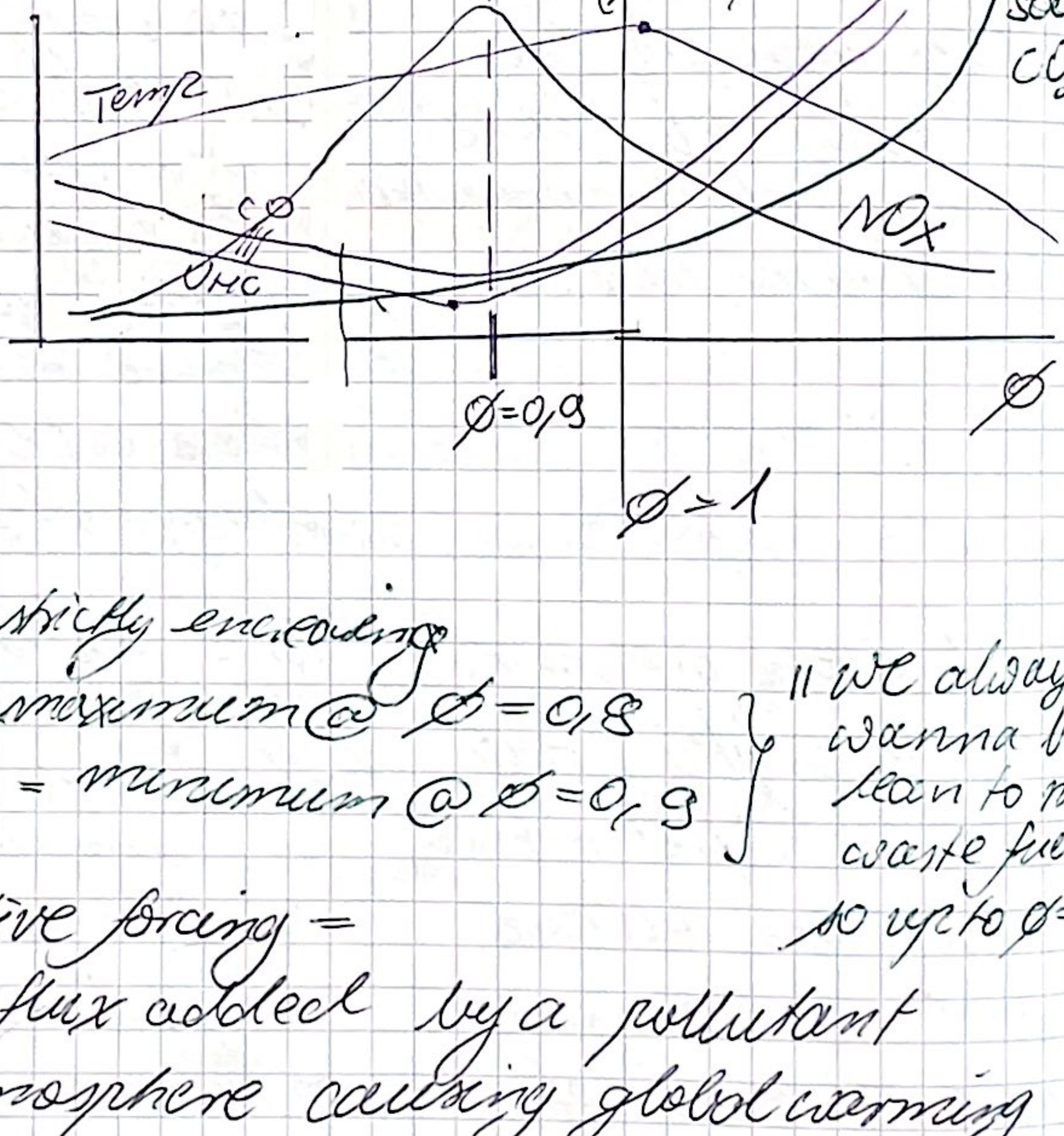
(10) Emissions

1. LTO cycle → max fuel flow @ TO, max NOx @ TO

" NOx & soot production decreases with low thrust, while CO & UHC rise with decreasing thrust"

$$\frac{\text{gToxic pollutant}}{\text{kg fuel}} = EI$$





(CO_2 ↘) SOOT = strictly encoding

NOx = maximum @ Ø = 0,8

CO ≡ UHC = minimum @ Ø = 0,9 } " we always wanna burn lean to not waste fuel, so up to Ø=0,9"

2. Radiative forcing =

radiative flux added by a pollutant in the atmosphere causing global warming

cooling effect for RF<0

- - - - ... Invariance of an isobaric process

- 2/3 of total +RF is due non-CO_2 sources
- 1/3 is CO_2 ($\frac{1}{2}$ due to contrails)
- CO_2 lifetime = 750 - 1000 yrs — affs that it decays or rain
- soot lifetime = 7 days — settles due to gravity

- aerosols can have -ve RF: SOx has "strong" -ve RF. Soot may have but low confidence.
- Soot is carboneous nanoparticles ("smoke") aggregated (chemically bonded) and or/ agglomerated (physically bonded — VDW).
  - mostly carbon & few hydrogen atoms
  - 10-50 nm diameter

From 1960 - now we've reduced soot significantly. Still 16g every yr is emitted during LTO cycle (remember — highest thrust)

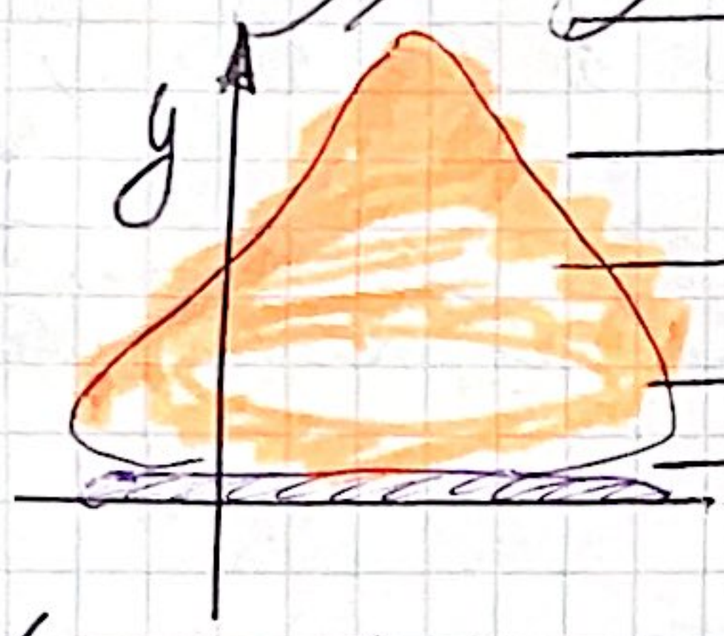
Soot is cancerogenous and toxic (like smoking)

Soot is the contrail nuclei (just like any aerosol). If reduce 90% soot, then it can halve the global RF.

In RQL, soot is mostly poluced in (R), close to the fuel spray nozzle. In (2), it gets oxidized so they burn completely before they're ejected. Soot can be removed by thorough mixing and preventing rich pockets.

3. Overview of soot formation

McKenna:



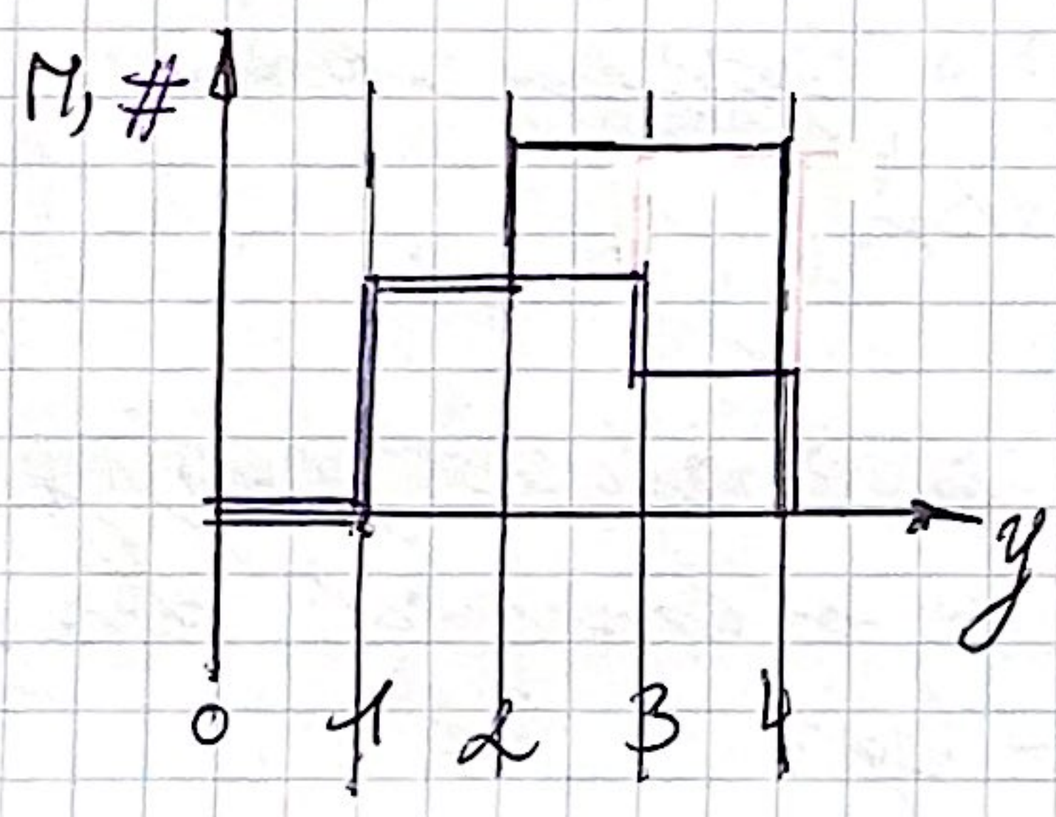
- oxidation
- agglomeration
- surface growth/aggl.
- soot inception
- PREcursor formation ①

① soot inception increases the # of soot particles AND mass

② growth → mass increases (not #)

③ agglomeration → # decreases

④ oxidation → mass AND # decreases.



M = mass total

⑤ Diesel soot formation $\Delta S < 0$ (agglomeration/aggregation) and $\Delta H > 0$ (endothermic), ~~so only spontaneous @ high T temps.~~

→ It's entropy driven, kinetically controlled: it's much more production than what can be predicted thermodynamically.

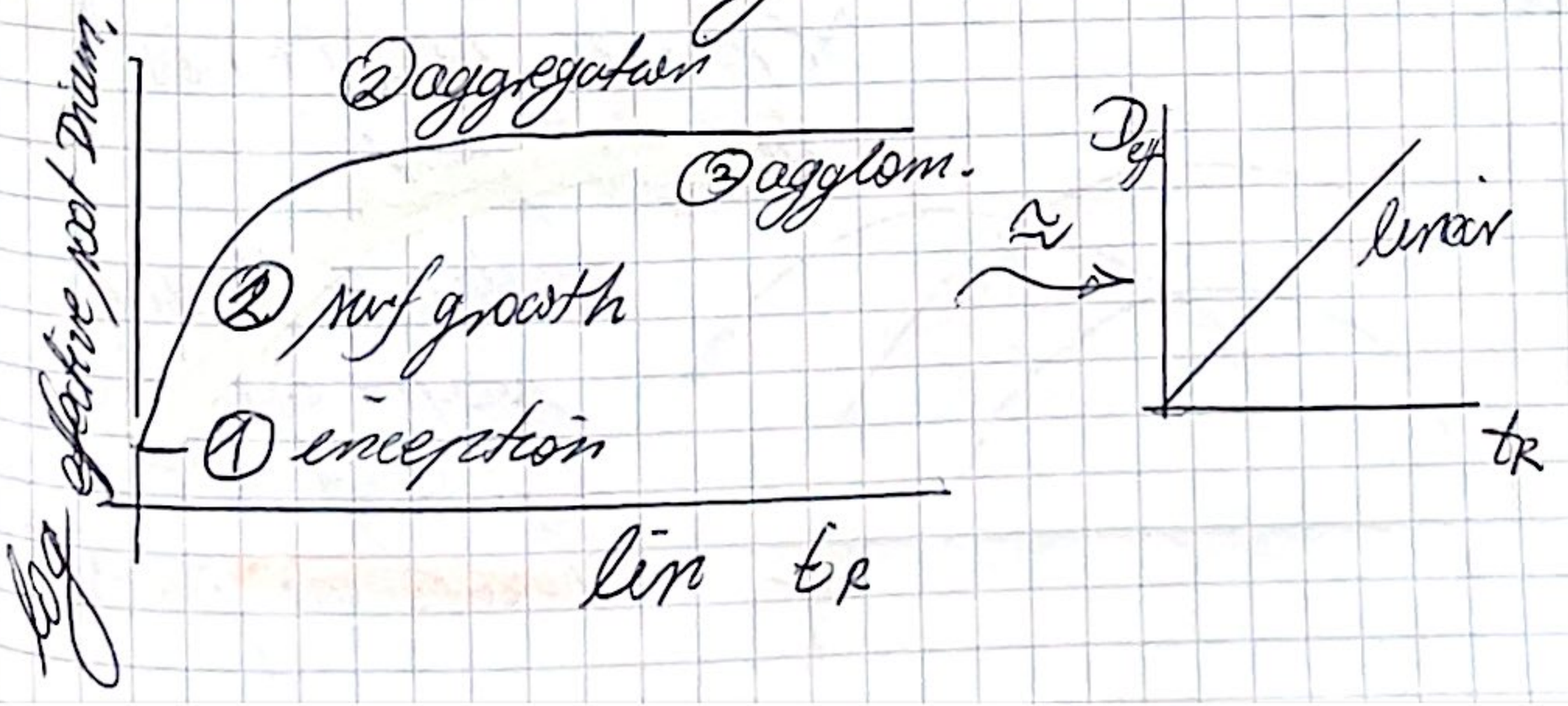
① key molecule for soot formation is Acetylene C_2H_2
It's known to polymerize @ high temps, most abundant intermediate species in hydrocarbons combustion, polymerization catalized by hydrogen.

Acetylene is the reactant for benzene formation so it points formation of so-called PAH molecules and their radicals thru the HACA mechanism (PAH = polycyclic aromatic hydrocarbons). PAH & it's radicals are thus responsible for soot inception

More precisely, inception happens thru reactions between stable PAH molecules & unstable PAH radicals.

② Surface growth is when C_2H_2 molecules react thru HACA with a soot particle — aggregation → chemical growth - the product soot particle has + = 2 C atoms.

③ Soot loves long residence time



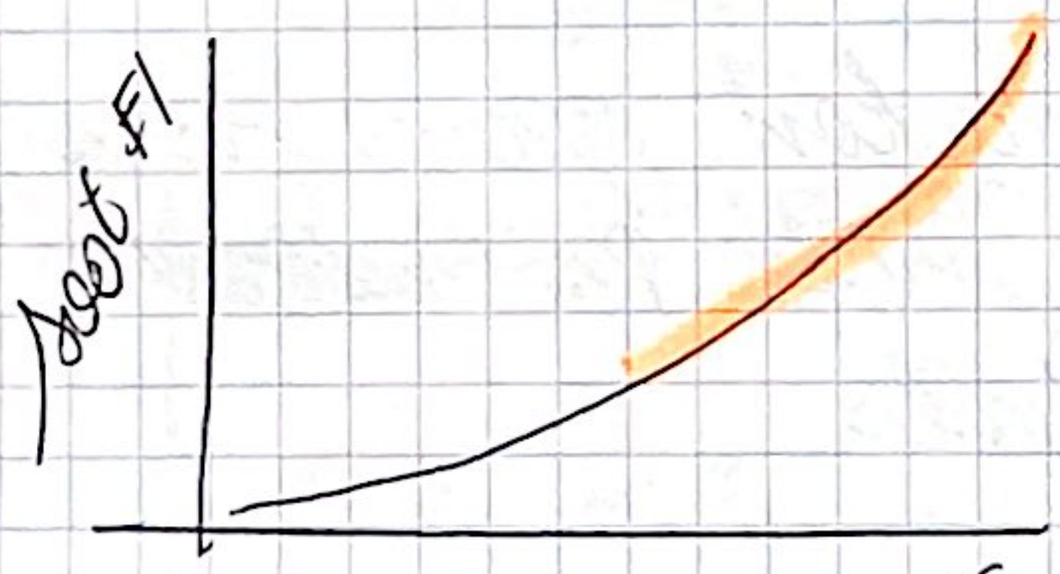
④ At the exhaust of the flame or en leen region, soot particles oxidize with O_2 and OH. The products are usually CO/CO_2

Oxidation rates of soot are currently being researched. Nowadays $\dot{\omega}_{soot} \approx \dot{\omega}_{graphite}$ though not fully correct because soot contains H while graphite doesn't.

4. Factors affecting soot emissions:

— t_R, T, P, ϕ, fuel type, presence of mixing

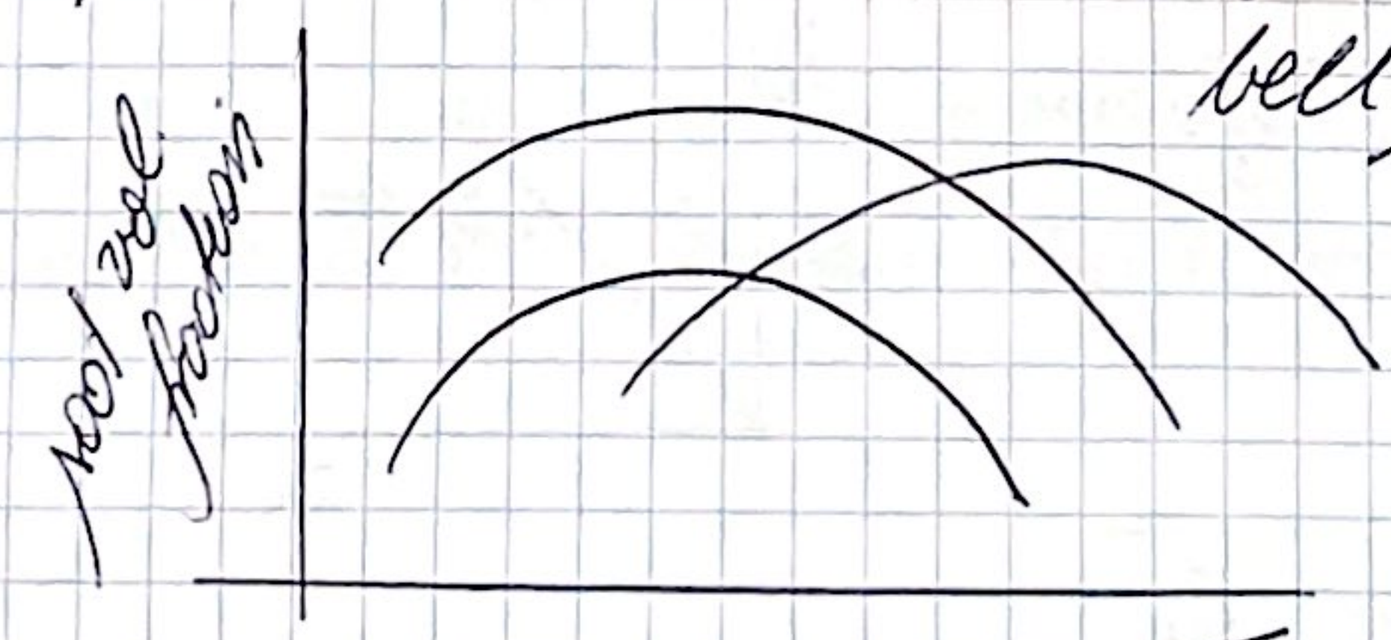
a) soot (ϕ)



@ higher ϕ, the flame luminosity is higher — it's a direct indication of soot concentration

ϕ monomer size ↑ as ϕ ↑ which encreases surface reactions so more soot (encrease of monomer size, not polymer)

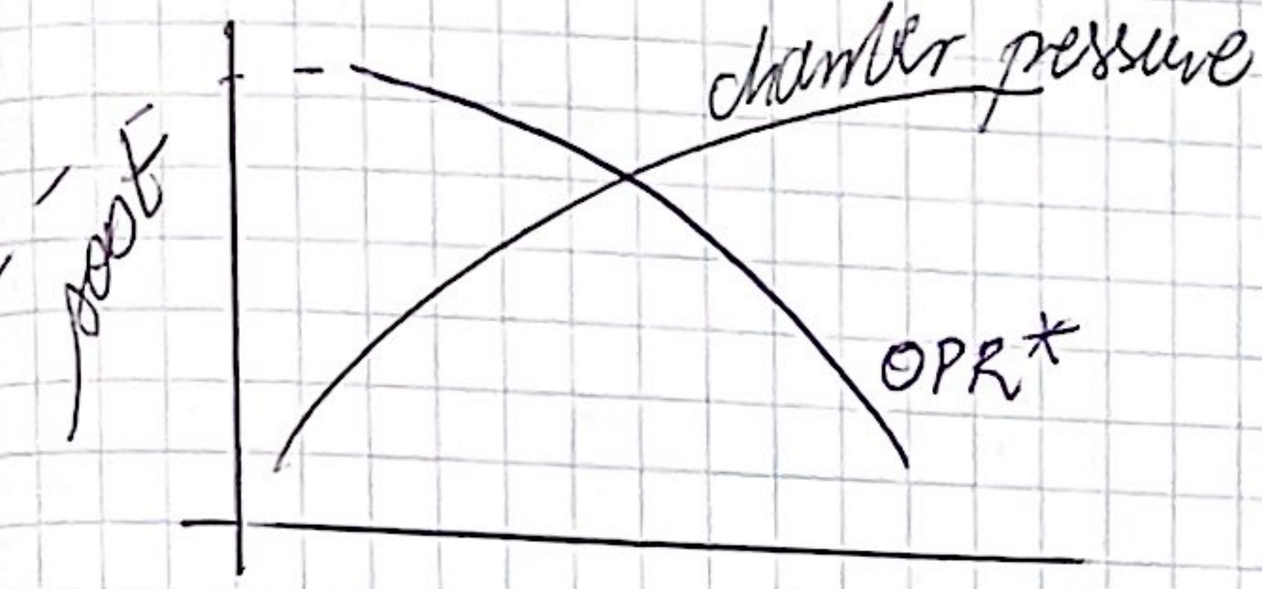
b) soot (T)



∀ fuels soot (T) is bell shaped

"the bell curve shape is a direct effect of the oxidation process"

c) soot(P)



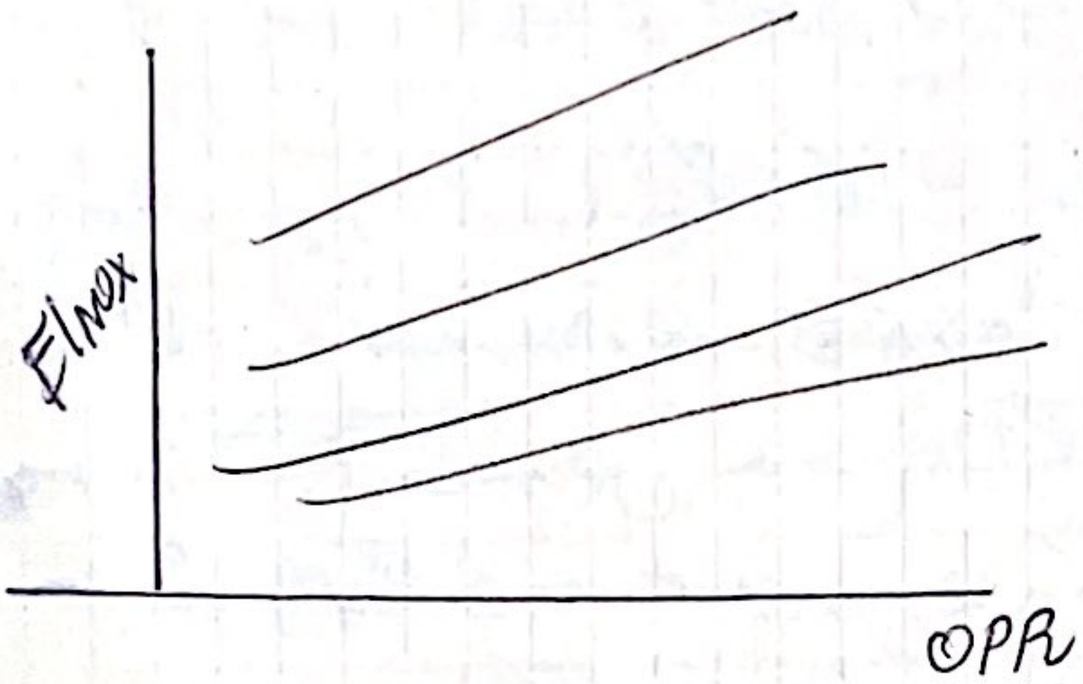
from luminosity you can't really tell although I a relation

- kinetics becomes faster & high collision rate (agglomeration - physical) @ high pressures

* why OPR↑ ⇒ soot ↓ ? cuz ↑ OPR ↑ @ high OPR ur cc temp ↑ and you're usually on the right-hand-side of the peak so you fall back to the bell curve.

5. Soot Emission reduction techniques
   - SAF (↓ of 30% - 50%)
   - cc optimization (lean burn)
   - H_2-fuels (0% soot but NOx ↑↑)

6. NO_x vs. OPR ($\sim T$)



7. NO_x formation mechanisms → note (N_2O is not NO_x)
- Thermal (Zeldovich), in
- Prompt (Fenimore)
- The N_2O mech
- The NNH mech.
- fuel NO_x ≠ Prompt!

a) Zel'dovich NO_x — set of 3 rxns proposed by J. Zel'dovich. Occurs @ high temps & t_R. Molecular N_2 & O_2 dissociate to form the following

1) $N_2 + O \rightleftharpoons NO + N$ } due to Zel'd.
2) $O_2 + N \rightleftharpoons NO + O$ } ← preferred if $\phi < 1$; big Ea!
3) $N + OH \rightleftharpoons NO + H$ ← due to someone else

preferred if $\phi > 1$

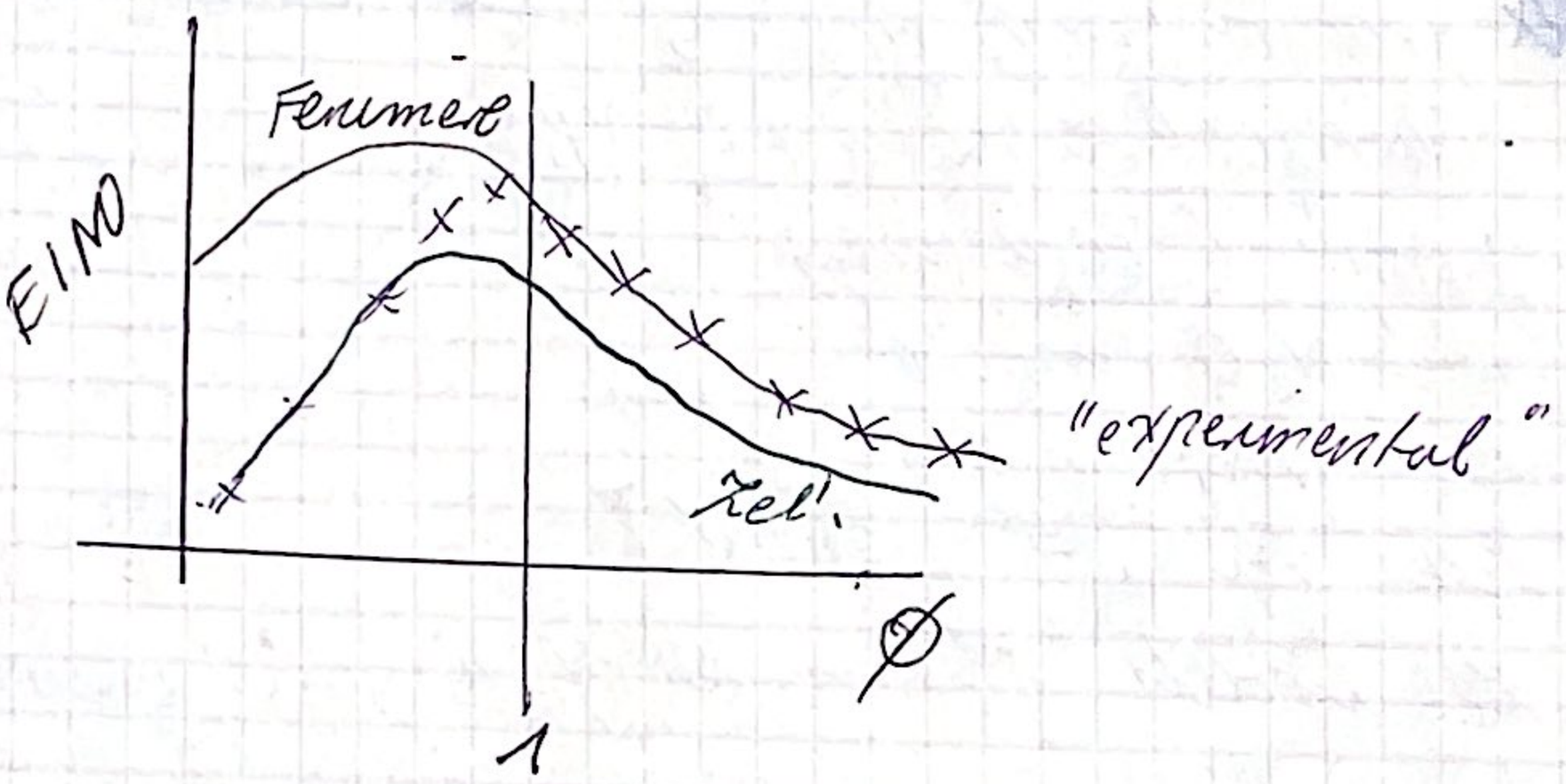
b) Fenimore NO_x — Fenimore noticed NO_x formation @ low temps & low t_R — this was not expected from Thermal NO_x: he proposed molecular N_2 react with hydrocarbon radicals to form cyanide:

$$N_2 + \underbrace{CH}_{\text{the "prompt" in Prompt } NO_x} \rightleftharpoons \overbrace{HCN}^{\text{cyanide}} + N$$

, fairly low Ea!

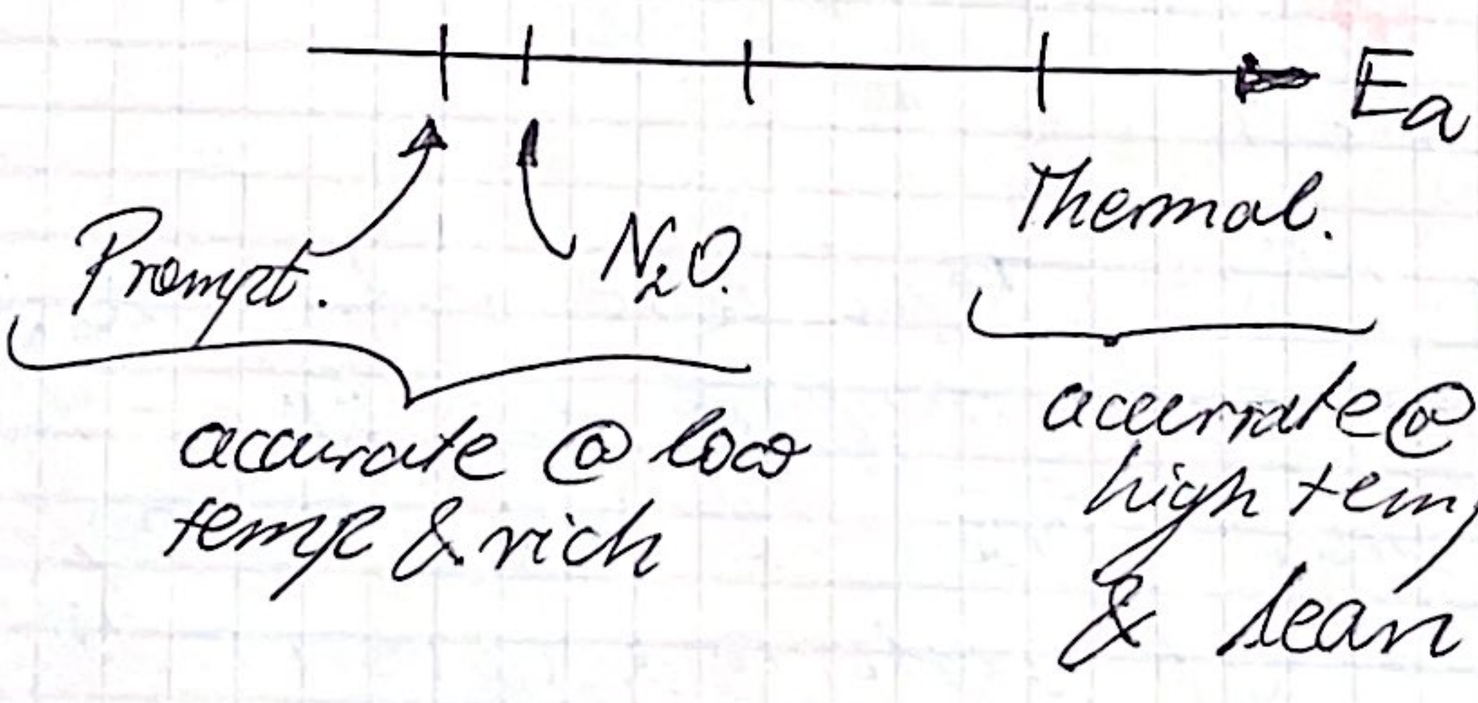
the products then undergo rxns to form NO.

the CH radical forms from acetylene C_2H_2 which only forms @ rich (recall soot vs ϕ "$\frac{|}{|}$").
This means that @ lean ∃ little CH·, so Fenimore does not contribute to overall NO_x.
Also the opposite holds → @ rich Thermal NO formation is not a great model & @ rich Fenimore is much better.



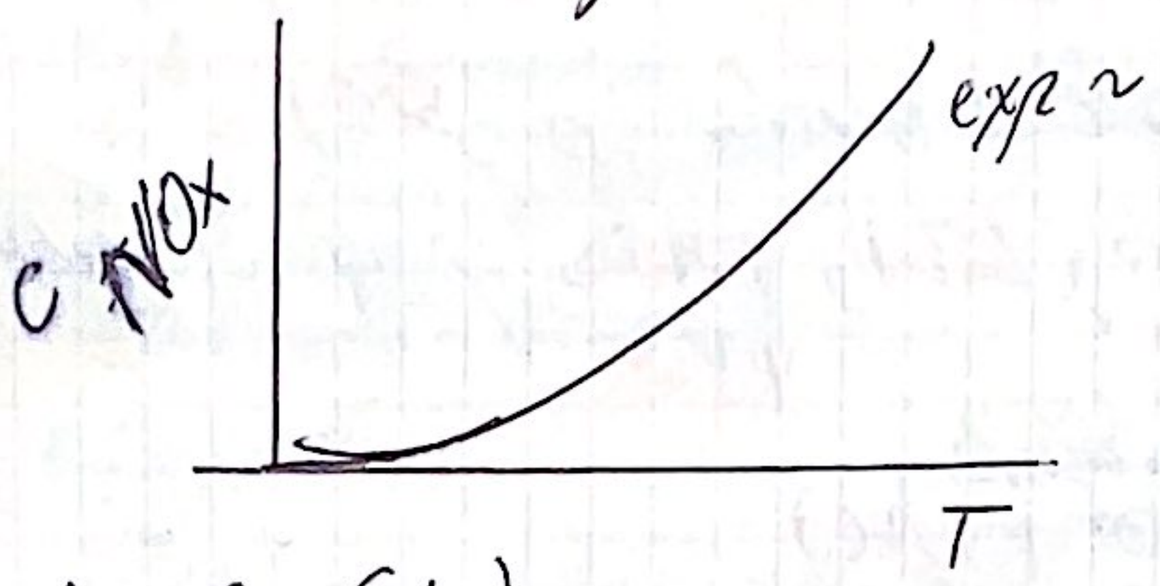
c) The N_2O mechanism is most accurate @ low temps due to low Ea.

Quick Summary:

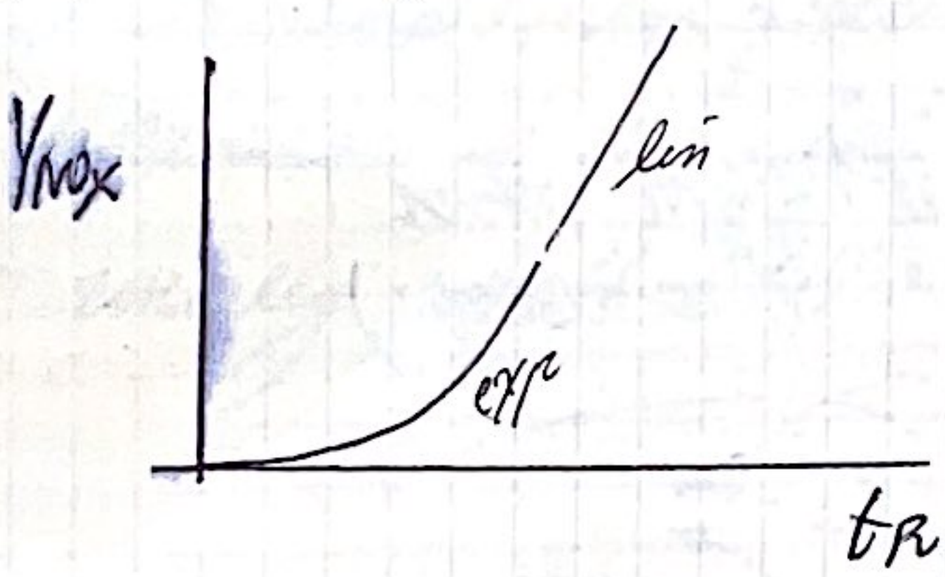


8. Factors affecting NO_x (literally same):
- t_R, T, P, ϕ, fuel, mixing

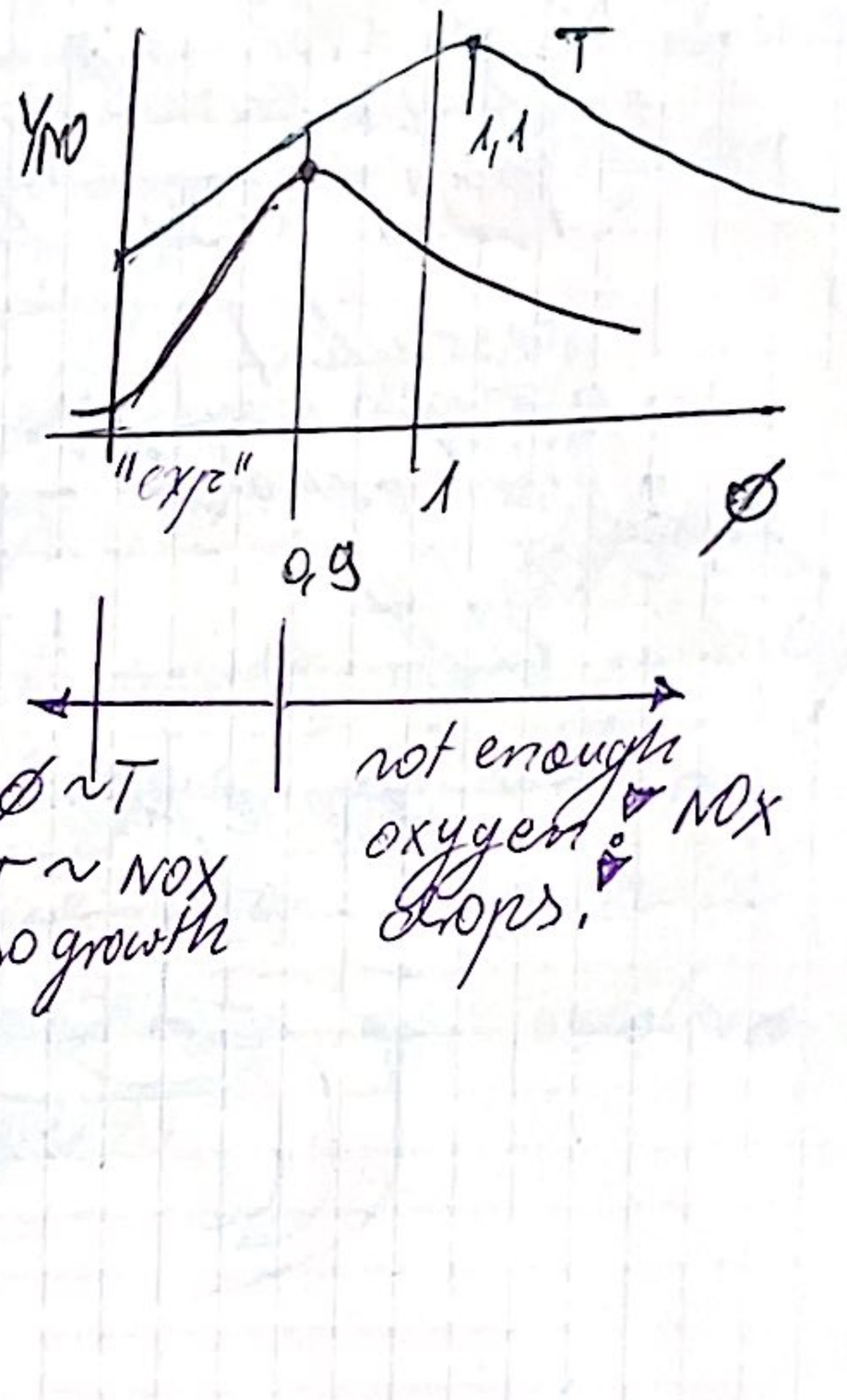
a) NOx (Temp)



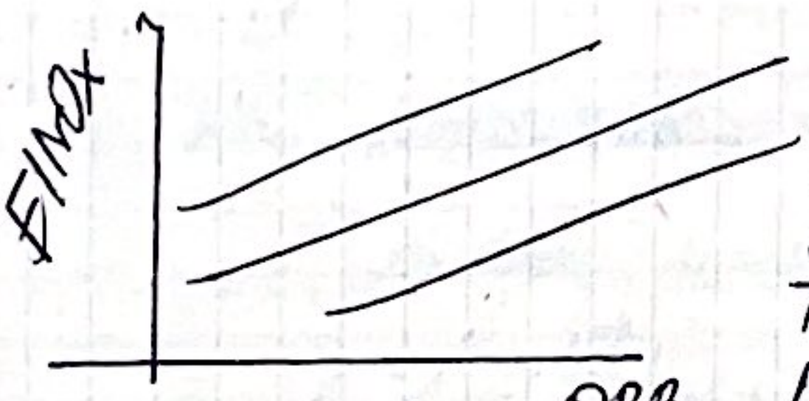
b) NOx (tR)



c) NOx (Φ)



d) NOx (OPR)

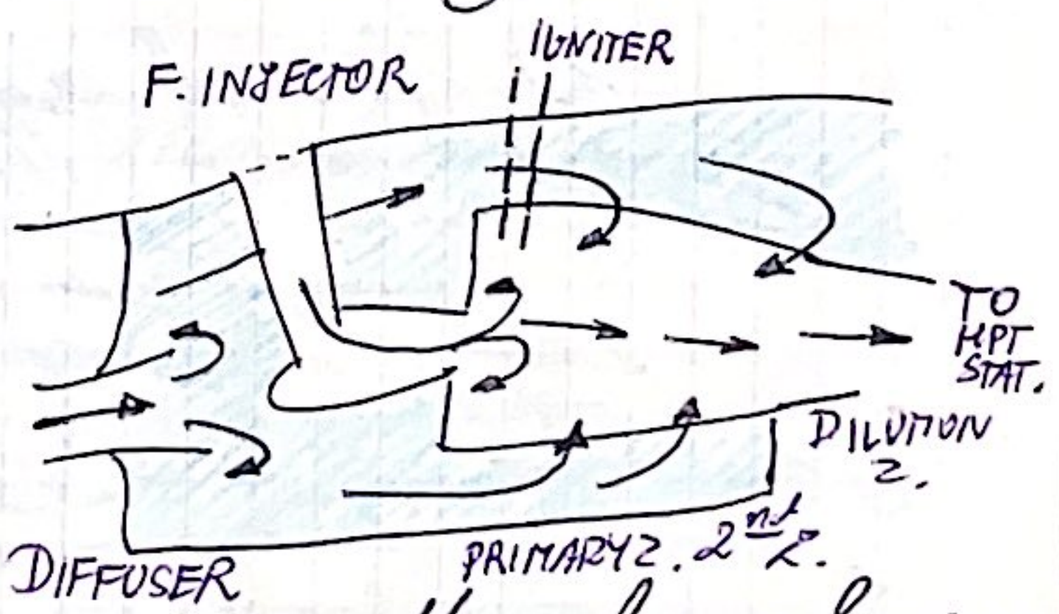


9. NOx reduction techniques:

- temperature control (RL, ..)
- addition of diluents (steam, water, gas recirculation)
- post combustion emission treatment (only for land turbines) - filtering

(11) Aero Engine Combustor

1. Chas of a typical combustor:

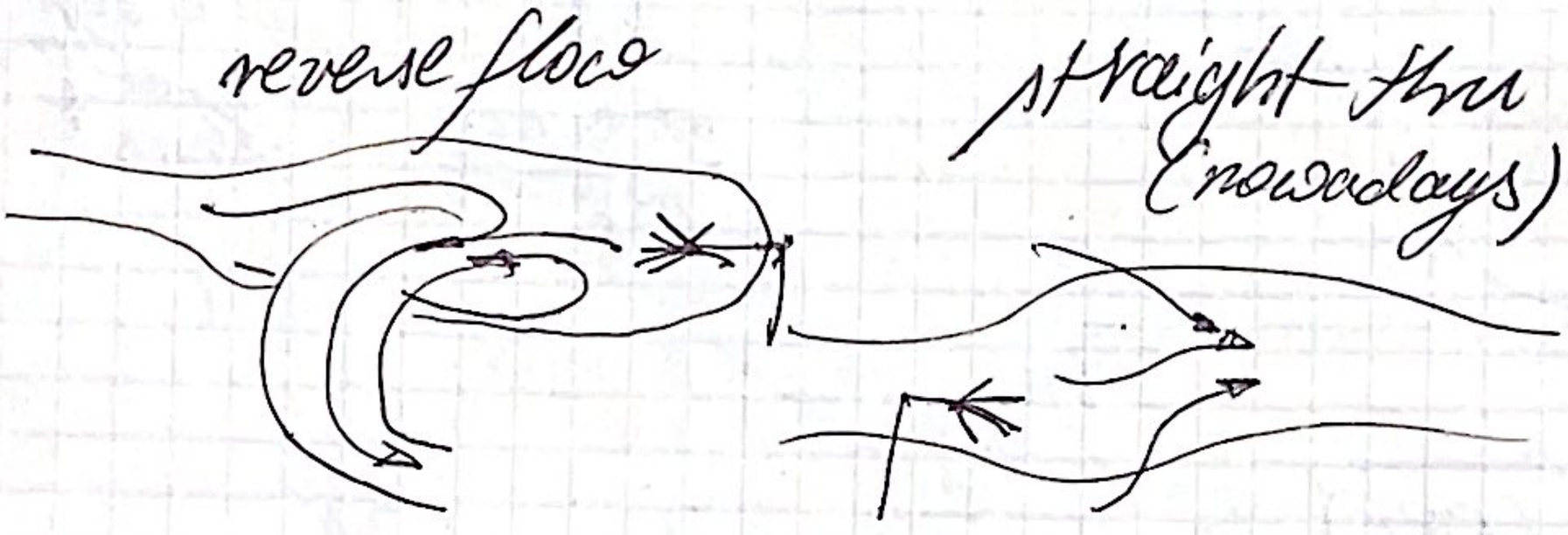


- primarily turbulent
- spark once, then self sustained
- nearly p = cont
- small volume & mass
- residence time @ loc nox small ~5 ms
- should be insulated/ adiabatic

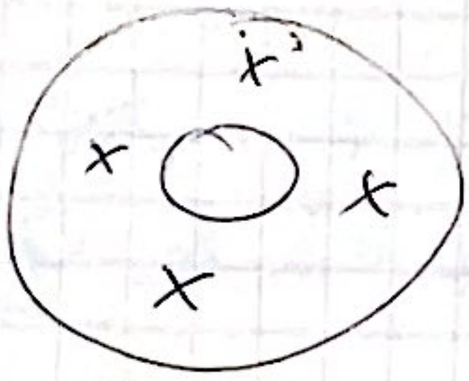
— combustor types :

- conventional : single annular cc (SAC)
- RQL, lean burn, LDI, TAPS, staged (double annular) LPP
- use of catalysts / inhibitors
- dble annular combustor (DAC)

2. cc config



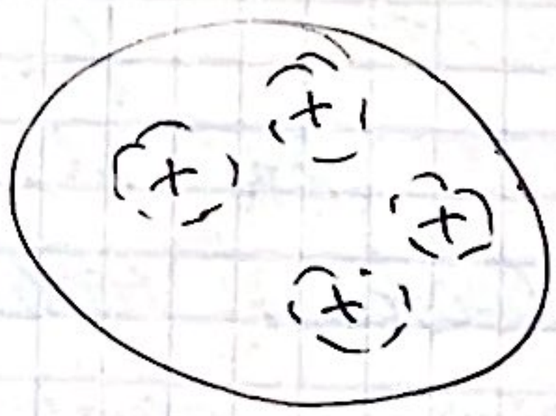
annular



can



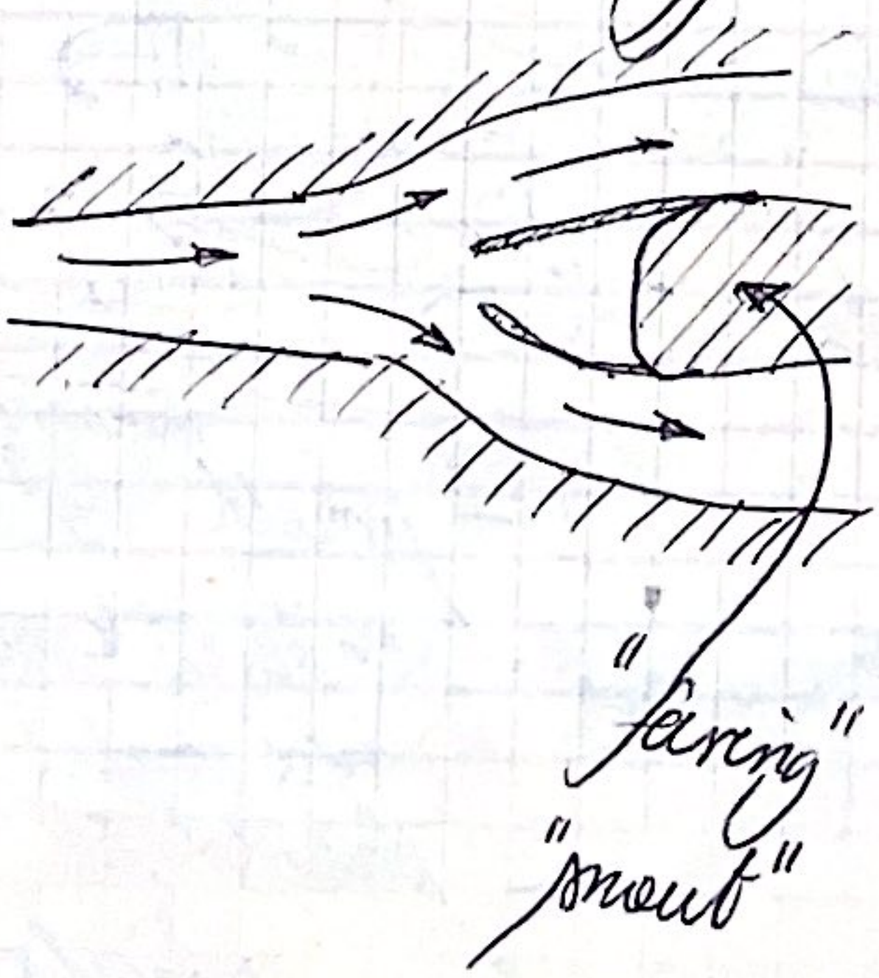
can-annular



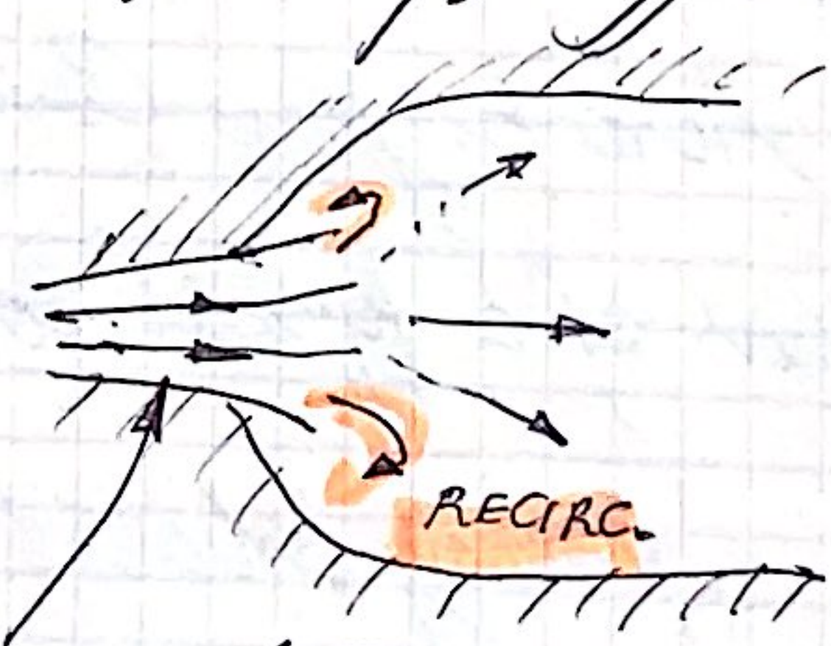
○ = liner
○ = casing
x = ff inlet

3. Air diffusion

i) faired diffuser



ii) dump diffuser



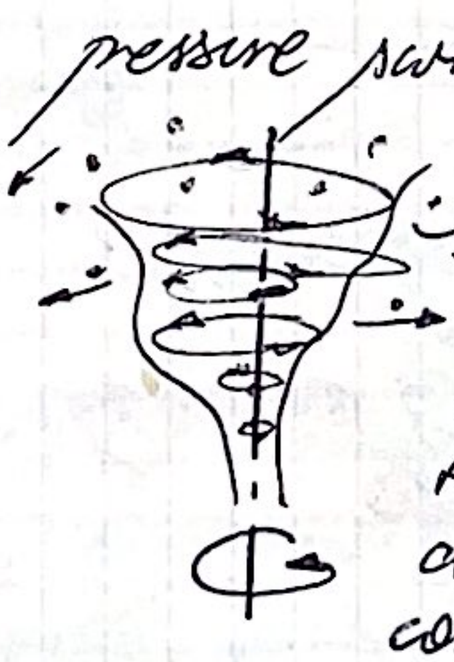
- long, smoothly diverging inner & outer walls ("fairing separates the annular passage(s)
- wall-bounded, attached flow decelerates gradually separation is avoided
- usually small TBJs

- short pre-diffuser followed by sudden area increase (dump) into an open cavity
- flow deliberately separates @ pre-diffuser exit, creating a free shear-layer that diffuses around a large comer-recirc. zone
- used in most modern engines.

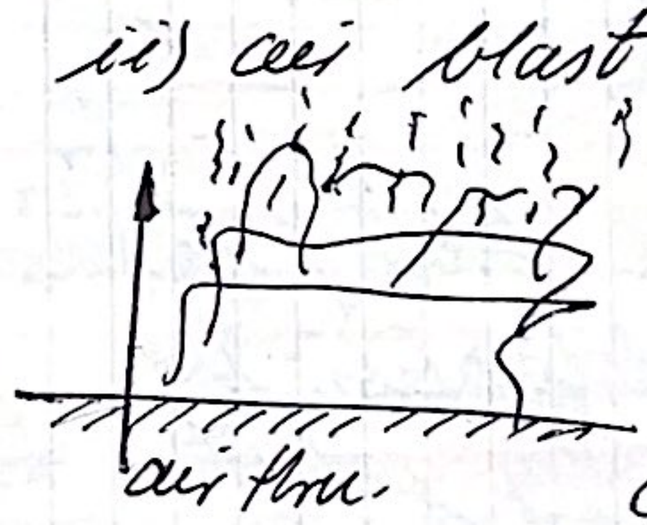
4. Fuel Injection

a) WRT atomization mechanism

i) pressure swirl

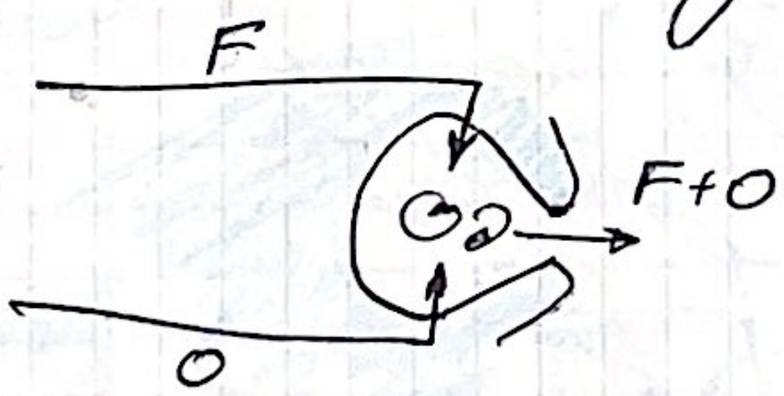


ii) air blast



b) WRT mixing type

i) internal mixing

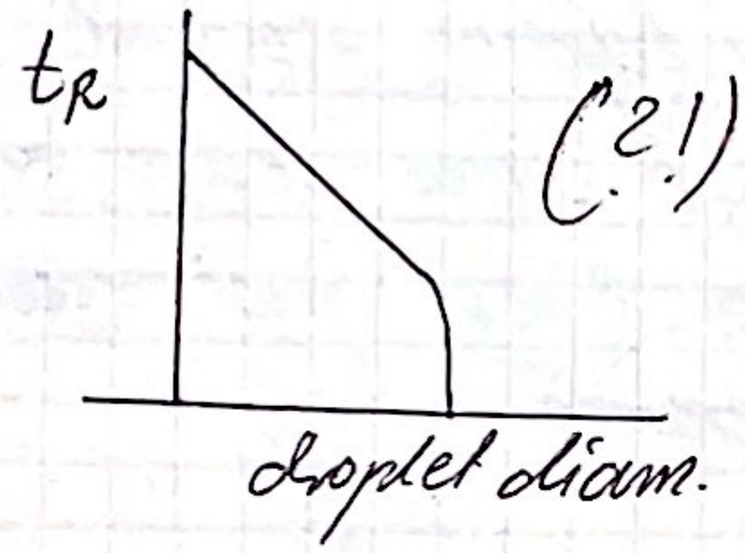


ii) external mixing

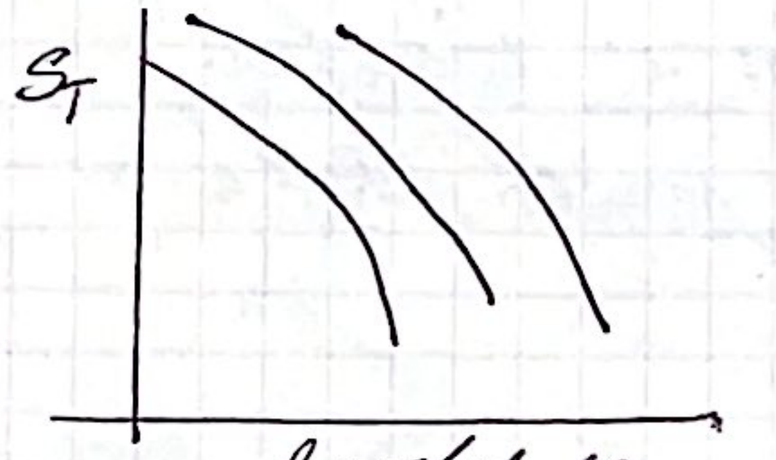


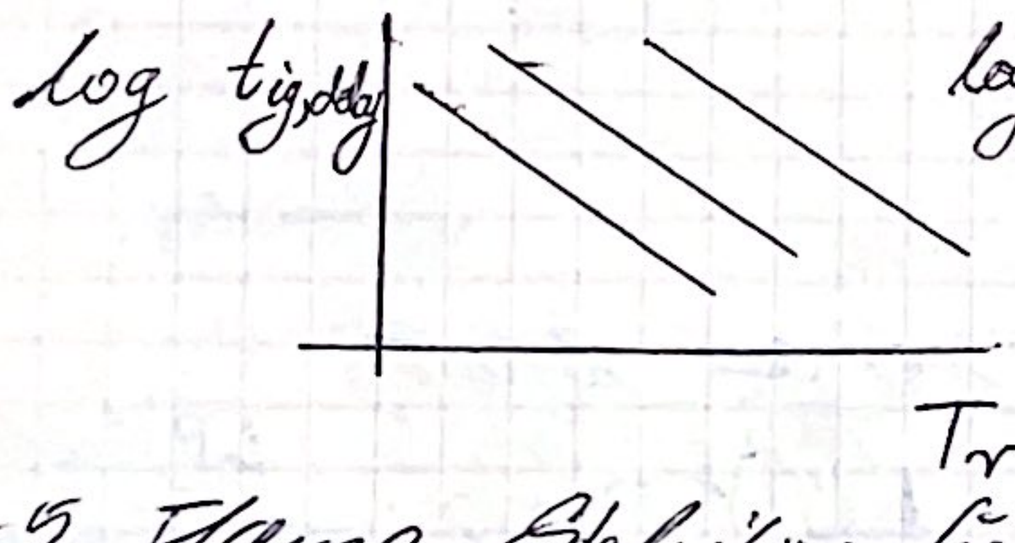
AD droplet diameter, flame speed & residence time:

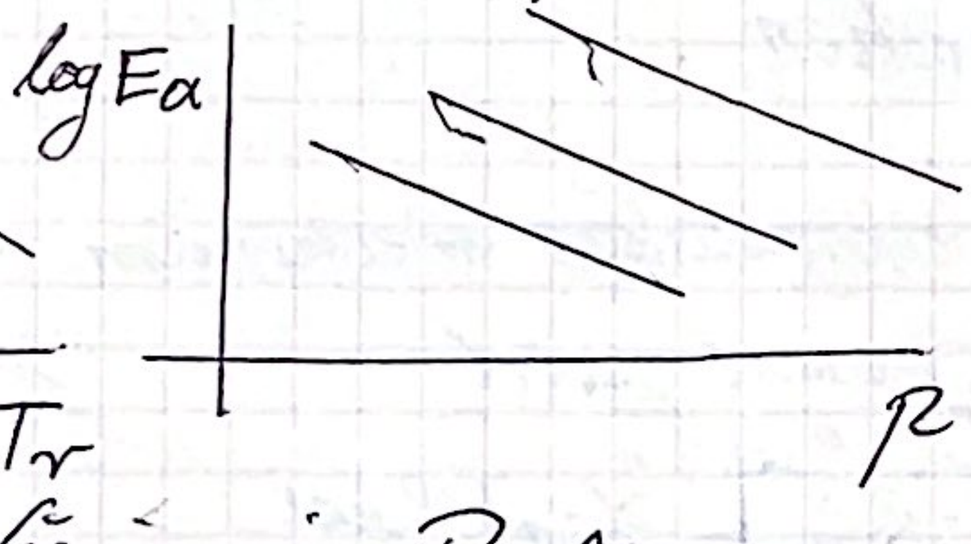
Notice that the bigger surface area/volume ratio, the faster evaporation so smaller t_R. Find $\frac{A}{V} = \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = \frac{3}{r}$, so if $r \downarrow$, then $t_R \downarrow$. Now, $t_R \sim \frac{1}{S_L} \Rightarrow S_L \uparrow$



(21)

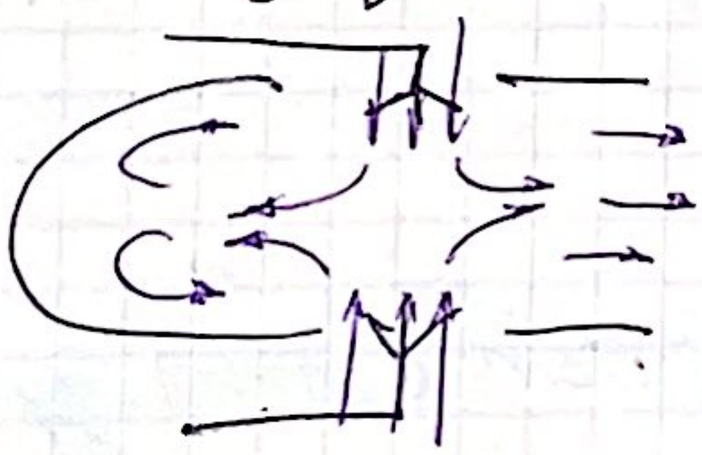






5. Flame Stabilization in P-zone.

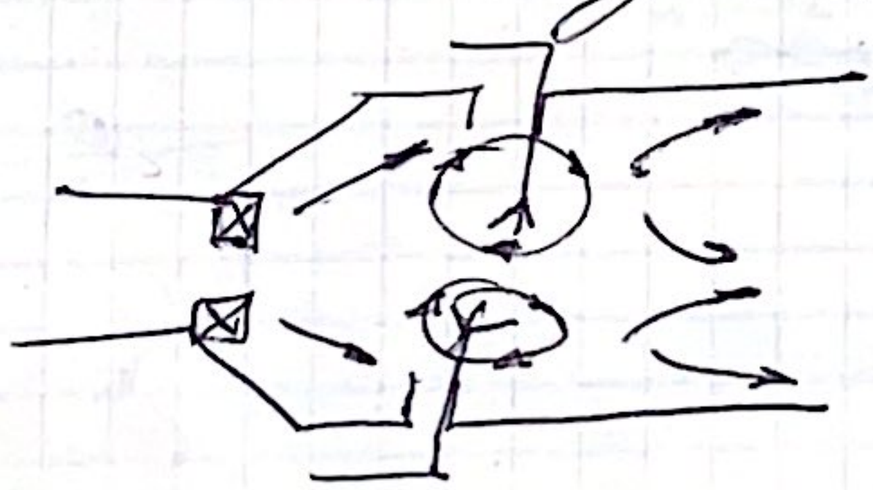
i) Stabilization by opposing jets



ii) Stab. by swirling jets



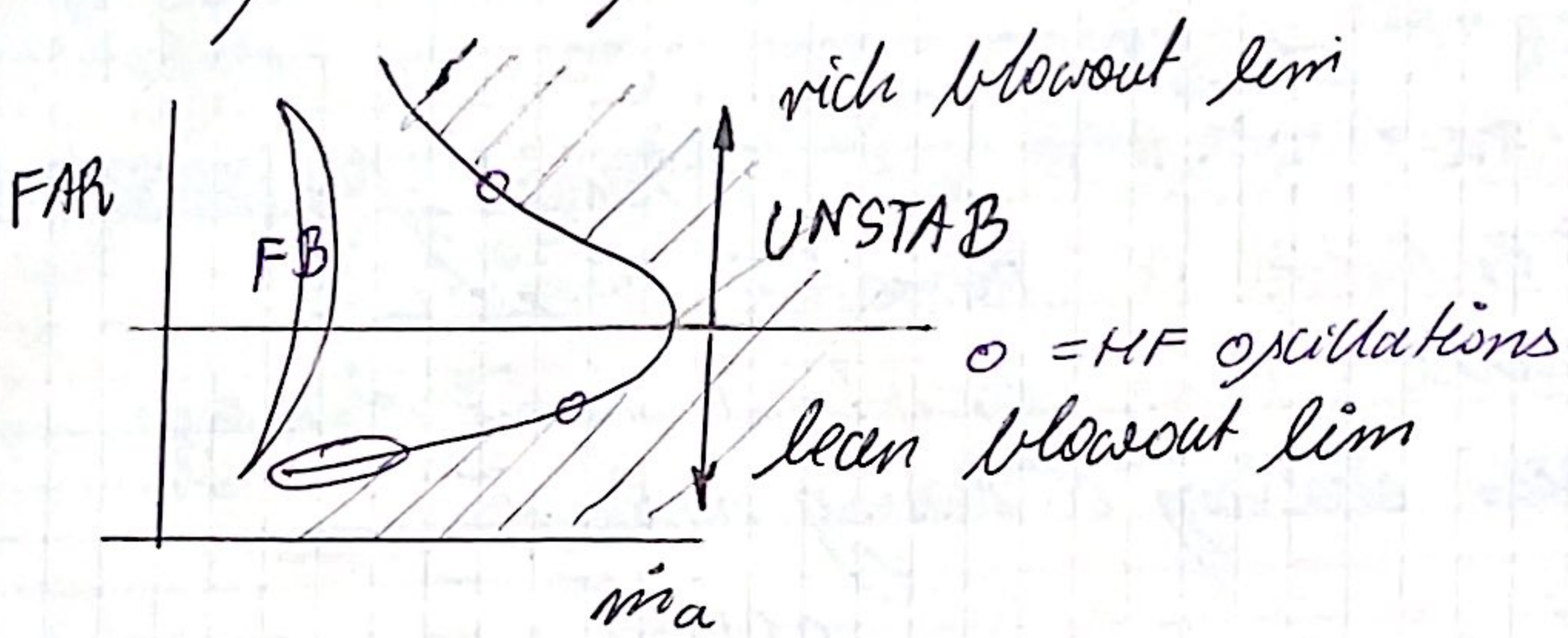
iii) By secondary injection



SWIRLER TYPES:

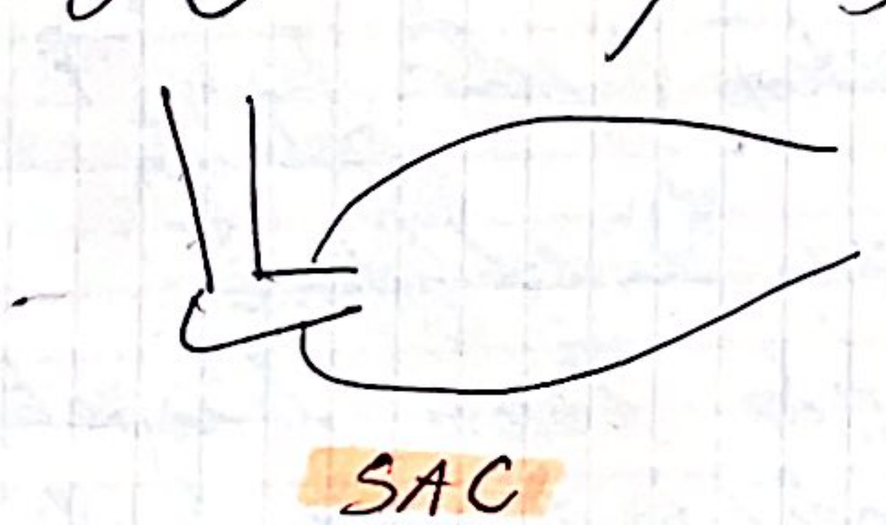
- AXIAL
- RADIAL

6. CC oper envelope



7. Combuestor staging:

- can improve combustion efficiency by enhancing the fuel-air mixing (less Diam → less t_R → less NO_x)
- staging can improve flame stability



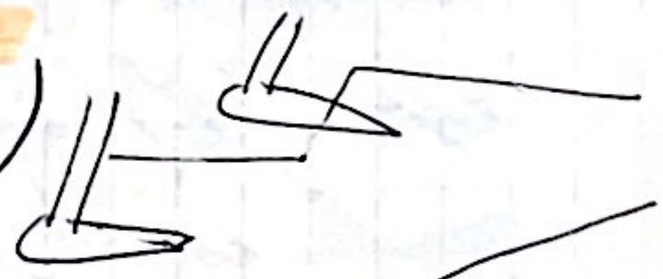
SAC



DAC

So DAC reduces NO_x but CO_2 increases!
(+ complexity & weight)

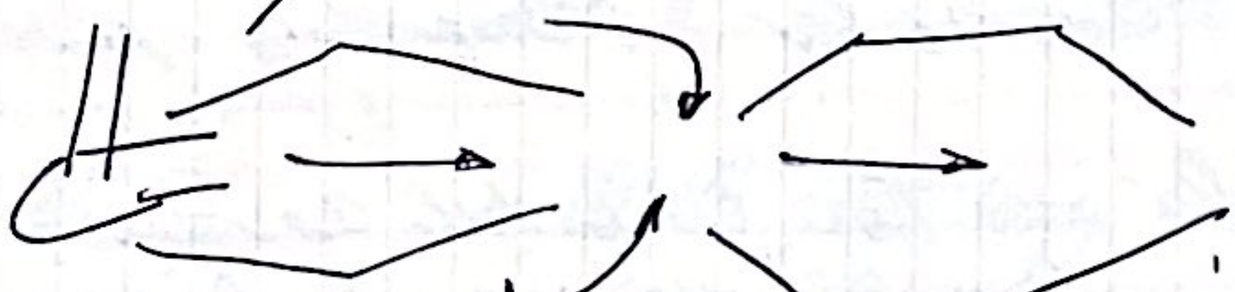
(double annular cc)



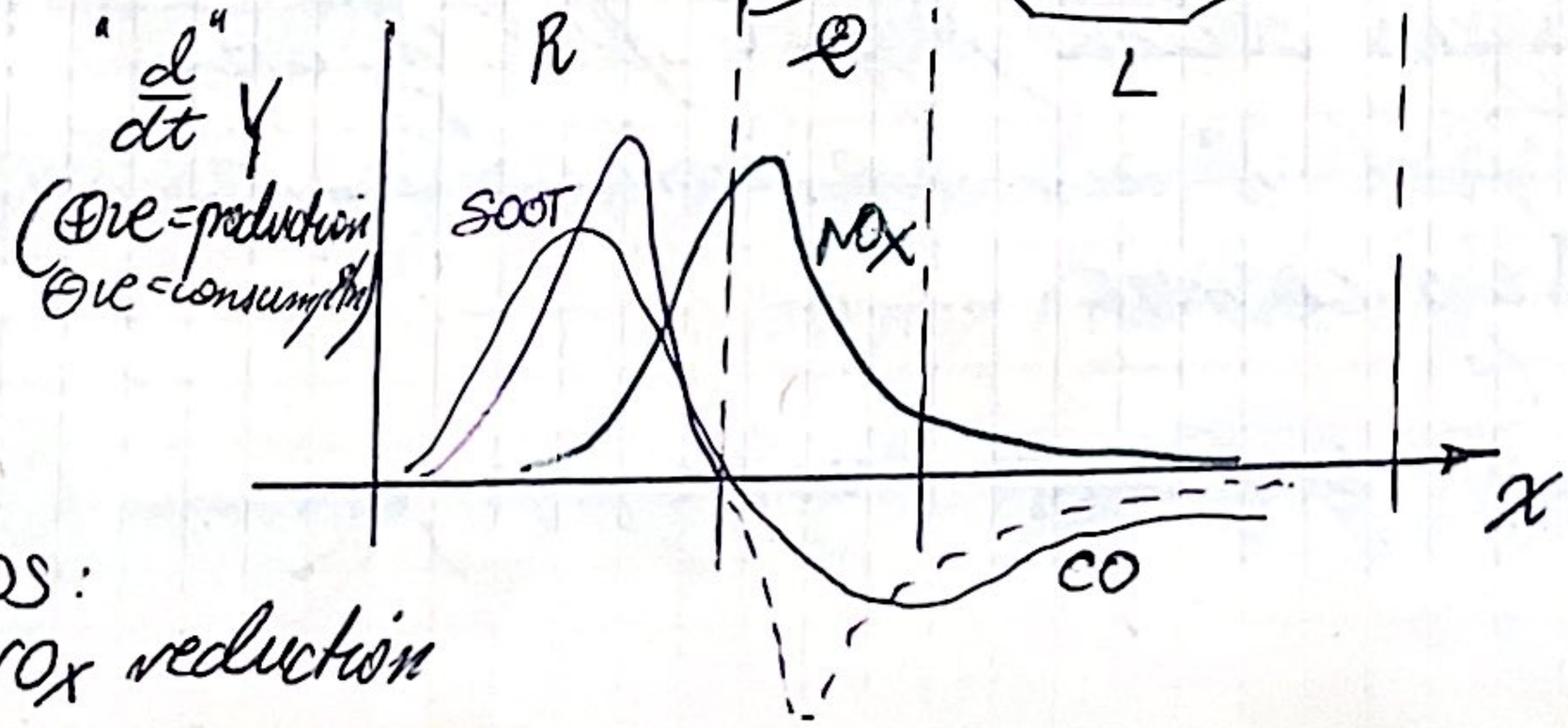
≈ 50%

ASC (axially staged combustor)

8. RQL - rich-quench-lean



R Q L



(R) QL produces lots of soot which is unconsumed!

"peak of soot emission is not @ peak of soot consumptn"

PROS:
- NO_x reduction

9. LPP – lean premixed prevaporized (soln to RQL high soot issue)

anti-soot
- lean : $\phi < 1$
- premixed : F & O are thoroughly premixed before entering cc promoting uniform cc.

anti-soot
- prevaporized : F is vaporized before mixing with air ensuring a homog mixture.

PROS:
- soot reduction

CONS
- they're premixed & lean so unstable (hypergolic, autoignition) & FB-prone (v. tall stability envelope) ↑ aux premix.

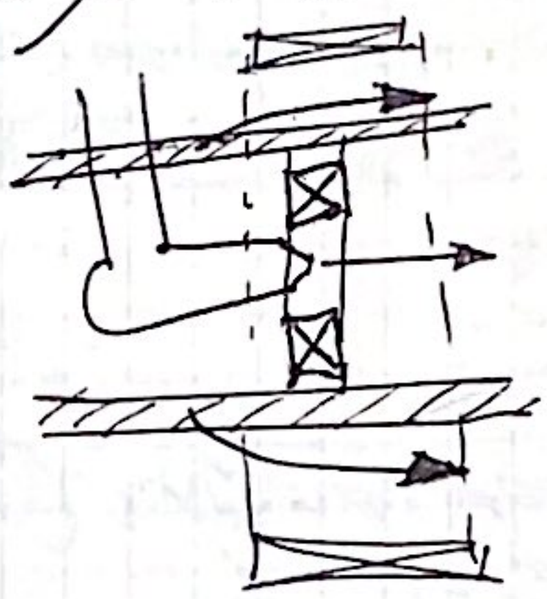
10. LDI – Lean Direct Injection (soln to LPP stability issues)

Separately injects fuel & air directly to cc @ very lean ϕ (close to lean blowout limit). Direct injection refers to the fact fuel is (X) injected to high T – high P mixture and instantly vaporized & combusted. ∄ dilution zone. Fuel & air are not premixed.

11. TAPS – two annular premixing swirler

- two annular – two concentric annular swirler passages allow staged fuel injection
- premixing : fuel & air are thoroughly mixed before entering cc zone.
- swirling flow – enhances mixing & flame stabilization.

en TAPS, liquid (!) fuel is injected with gas air to provide way more stability than LPP ~~LDI~~ and less soot & ~~NOx~~ than LDI / RQL.



	RQL	DAC	~~ASC~~	TAPS	LDI	LPP
TRL	9	9	≤5	9	≤7	≤5
FB risk & autoign. risk	L	L	L	M	L	H
stability	H	M	M	M	M	L
$EINO_x$	L	L	L	≪L	≪L	≪≪≪L mais !
EICO	M	H	M	H	H	M
EIUHC	M	H	L	L	L	L

↑ well established & "traditional"

↑ most promising cuz TRL = 6

L L — good emissions ≈ bad for stab ?

- ~~μ-MIX~~ (premix flame but with small t_R)
  - ✓ NO FB, less NOx (cuz less t_R)
  - X many injectors (interference + complexity) manuf & maint.

(R) Hydrogen Combustion I

1. We're encreasing efficiency thru TBF — 80% of thrust from fan, BP also reduces noise by lowering T_2.

2. What you require from cc
- low weight
- cost
- easy maintability
- relight
- wide oper envelope (Stability)
- fuel flexibility
- lowe emissions

...

3. ANNULAR

ADV	DADV
- less Area	- complex manuf &
- lighter	maintenance
- T = uniform	- no redundancy
- minimum Pwes	

CAN

ADV	DADV
- easy maint & manuf	- uneven Temp field
- redundancy	- heavy
- stable (interconnector)	- high Pwes

4.

	CO_2 effects	non-CO_2 eff's
fine scale location dependence	centrics	contrails: hours H_2O: hours / months
	NO	STRONG
contribution	1/3	2/3 ($\frac{1}{2}$ is ~~1000~~ contrails)
confidence level	H	M/L

5. CO_2 reduction through: reduany TSFC, ↑ η

6. Factors affecting the choice of en. source/carrier:

- infastructure
- cost
- TRL
- availability
- Policies
- climate impact ...

7. Possible Scenario

ELECTRIC H_2 SAF

commuter, regional, short range } 1/4 em. → BATTERIES

med. r. } 3/4 emissions → FUEL CELLS

long r. → H_2 CC

SAF CC

for medium range aux H_2 tanks by to minimize A/V ratio, no long tanks & less pax lit.

radical transformation

drop in (easy replacement for kerosene)

Why SAF can be carbon neutral?

SAF is only CN over their full lifecycle — what's been absorbed by the plants can be dumped back in

SAF is a "drop in solution" cuz can be easily used in existing AC w/o significant mods.

SAF only reduces carbon footprint, not soot, NO_x etc.

Issues with SAF:

a) fuel composition & charts — even tho composition is similar to kerosene, it might not allow for the same engine characteristics (performance) (lubricators, relight conditions, ...)

b) certification & testing → difficult & cumbersome: must certify not only the fuel but the blend too.

c) cost → 10x more expensive!

d) low availability & TRL of certain pathways & feedstock (although ~~I~~ commercially mature solns — HEFA)

Pros of SAF:

a) Pathway towards carbon neutrality

b) "drop-in" solution — easy

c) similar LHV

8. So why hydrogen?

a) not enough SAF

b) Zero-emission potential & long-term sustainability

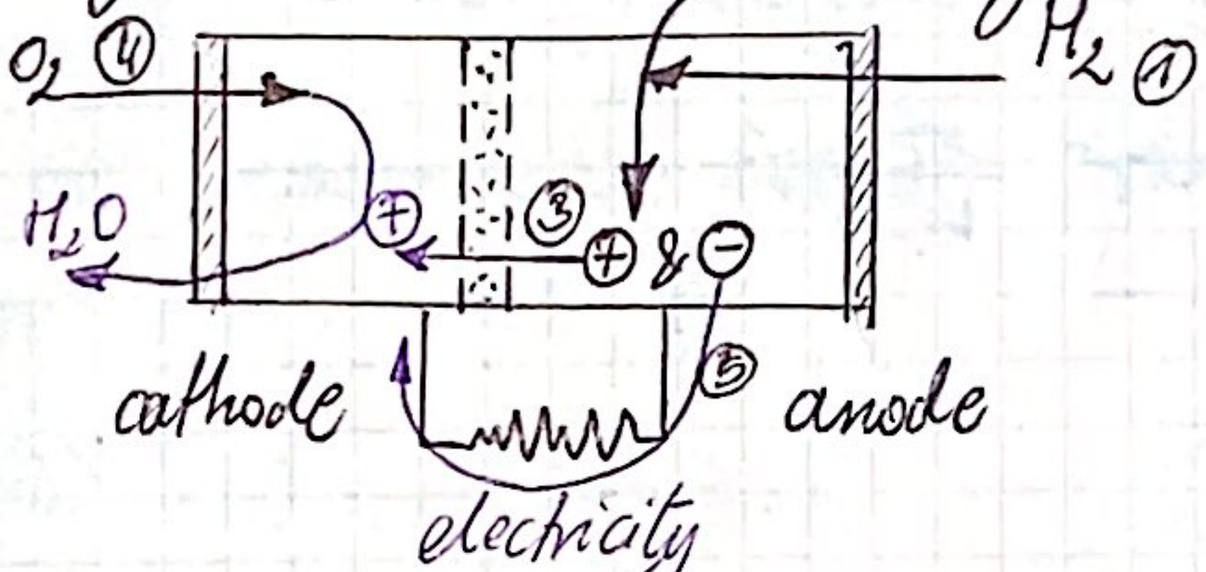
c) light & energy dense

d) versatile

e) declining costs & abundant in nature

→ can be used as energy carrier for fuel cells & direct CC.

i) hydrogen fuel cell



① H_2 enters @ anode

② catalyst breaks H_2 to protons & el-s.

③ protons move towards cathode thru one-way membrane to

④ connect with O_2 and form H_2O which is then removed

⑤ free electrons move thru an external circuit creating current

→ only useful @ low power, 50% efficient, up to 1kkm

ii) cc Hydrogen

H_2 is not a drop-in fuel! (CONS:)

$Le_{H_2} \approx 0,3$ ·1 higher diffusivity & reactivity : differential (@lean) diffusion & leakages

·2 higher flame speed : flashback, stability, dynamics

·3 higher flame temp : NO_x!

·4 storage & distribution : Kryogenic tanks, high P, pumps — need to pressurize LH2 to reach cc, so like in rockets except they need to work continously & must be reusable.

·5 certification — if not all components are compatible with LH2, it means a gigantic certification pocess

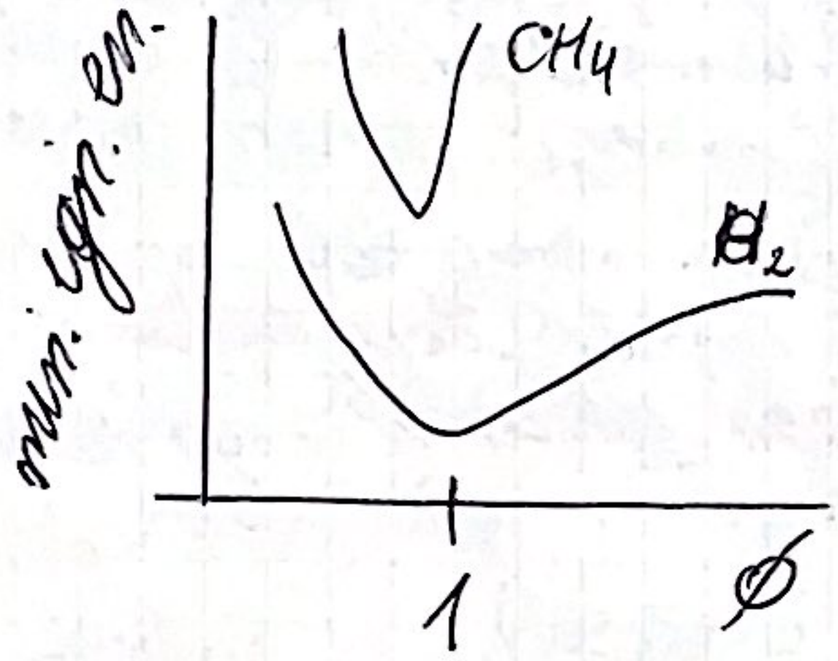
·6 infrastructure & transport

·7 safety (stability)

8. LH_2 not a dopen solutoni

10. Can LH_2 be stored ei oengis? Absolutely not! → must menimize $\frac{A}{V}$ to menemize vooliatori.

11. Safety of H_2:



flammability limit = ignition of H_2 occurs if H_2-content is below the Lower Flammability Limit (LFL) (ein ai – H_2 mixture) and above UFL. AND if an ignition source is present (then: hypergolic mixture)

→ So any ignition sources must be elemin-ted!

if no extenal ignition source is present, FO mixture may autoignite, as well — autoignition temperature (refer to the explosion diagram). For H_2 autoign temp > twice an for ~~for Ethy~~ kerosene.

12. Hydrogen Pros & Cons Summary

PROS	CONS
- no C-related emissions (soot, CO_2, UHC, CO)	- reactable - flashback prone
- ~~diff~~ high autoignition temperature	- high temps may lead to NO_x encr
- available (in nature & not only)	- certification burden
- versatile: fuel cells & H_2 combustion	- difficult storage, transport & distribution
- wide flammability limit	- high diffusivity - leakage
	- cost high

13. Hydrogen production:

- green H_2 → produced thru water electrolysis with electricity coming from renewable en sources.
- blue → comes from fossil fuels but the released carbon is captured & stored underground (carbon neutral).

(13) Hydrogen Combustion II

1. Flame which is premixed is extensionally unstable if the disturbance propagation rate is faster than the flame speed itself. The instability is caused by the flame itself.

2. The intrinsic instability can accelerate the flame & increase flame speed → HRR ↑ → burning rate ↑

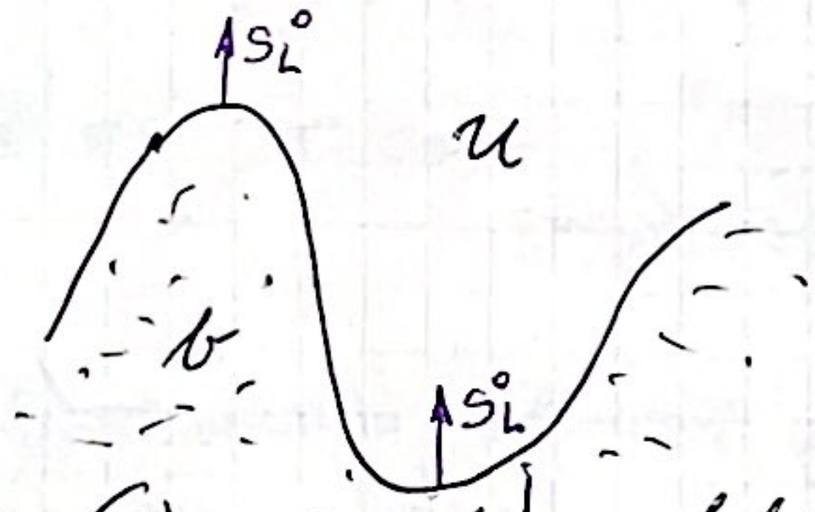
3. 3 types of cellular flame extensio instabilities

a) Thermo-diffusive instability

→ caused by preferential diffusion:

where $|Le_k - 1| \gg$ is big, i.e. when thermal & mass diffusivities differ significantly (do not confuse w differential diffusivity — different ways diffusivities between two (or more species) relevant @ small scales.

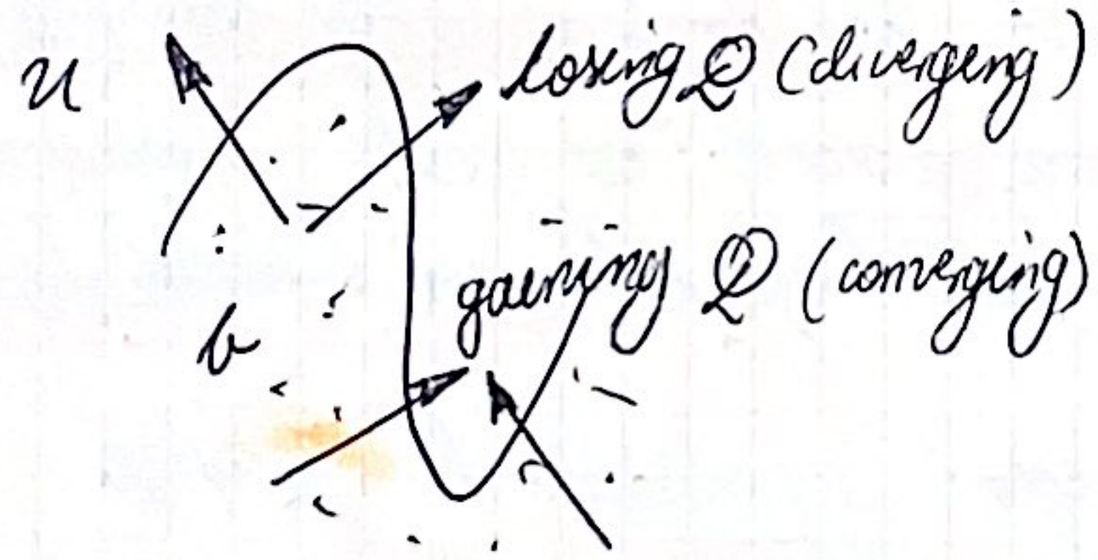
0. Starting point. determine Le and begin w a wrinkled flamelet



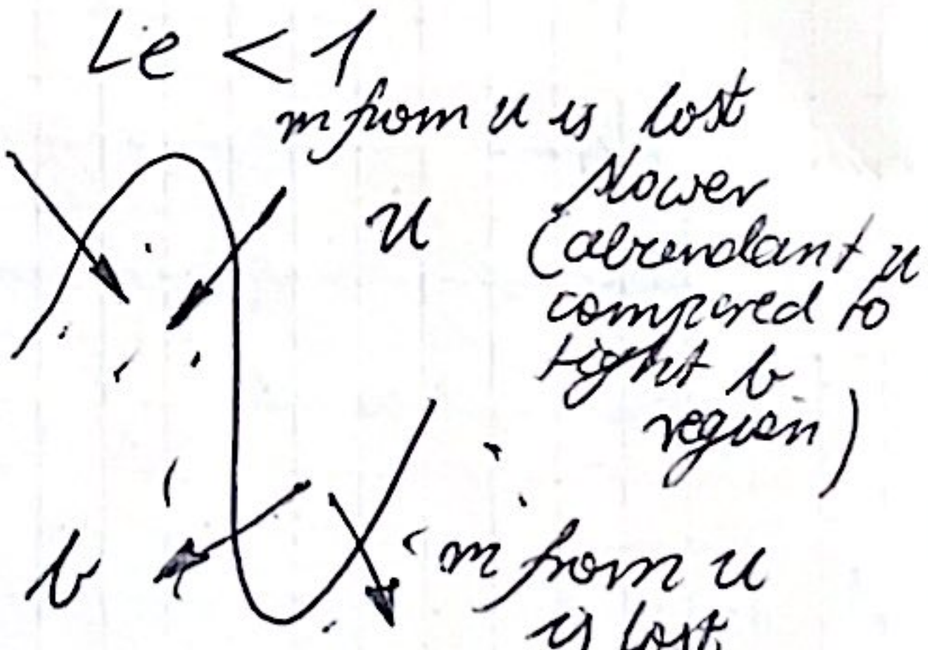
1. Based on Le (> or < 1), determine the dominant flux: $Le > 1 \Rightarrow$ thermal, $Le < 1 \Rightarrow$ mass.

2. Determine if you're losing or gaining* that q-tity (mass or heat) depending if you have valley or a hill. :

$Le > 1$



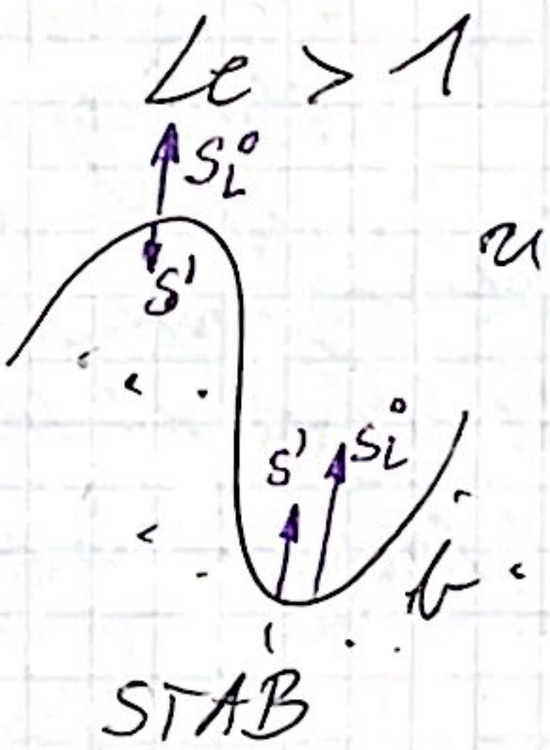
$Le < 1$

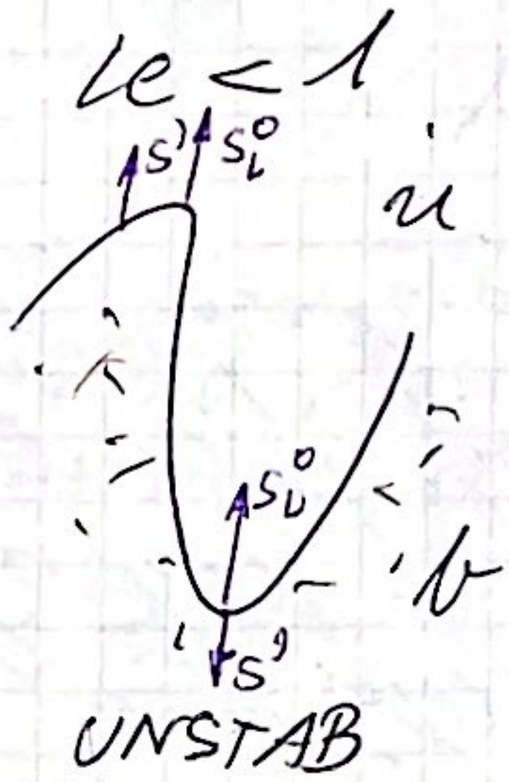


~~* if the u-region gains or loses~~

3. If @ is gained → Tad so S increased
[cools] [decreased]

If m is gained → Tad so S increased cuz u
[lost] [decreased]
burning @ richer [leaner] & so Tad increases
[decreases]





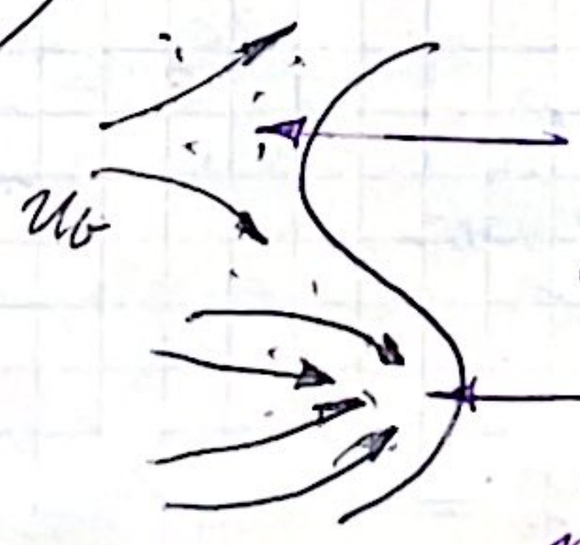
4. See when $S_L = S_{L0} + S'$ decreased & where increased & determine if flamelet gets stretched even further (unstable) or compressed (stable)

b) Hydrodynamic Instability (Darrieus-Landau)
→ assume ∞-thin flamefront; can be in gases too so idk why "hydro". Relevant @ large scales

0. Realize that $S_b < S_u \Rightarrow u_b > u_u$ so that $\dot{m} = const$. So ∃ a constant "pushing velocity" (momentum) from burned gases to unburned gases (burned "wins the balance cuz bigger").

1. Flow is subsonic

2.

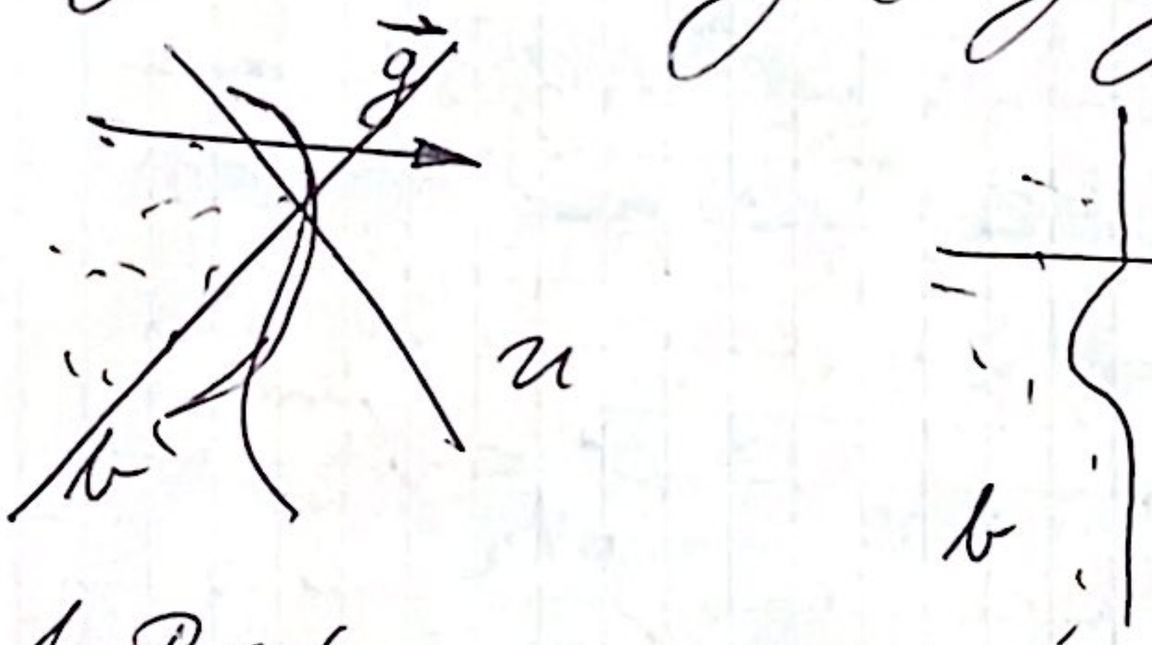


u_b decreases in magn. cuz diverging (nozzle) - doesn't push as hard to the right so valley moves left

u_b increases here (converging nozzle) so the bulge increases to the right

3. Overall result is destabilizing

c) Boyant enstability (Rayleigh-Taylor)



Relevant only if boyancy term ≃ chemical term

Usually not relevant in AE.

1. Due to gravity, the initial wrinkle magnifies — gravity pulls down (right) the heavy reactants while boyancy pulls the bubble more up (left) — unstable

4. Celleular flame enstabilities

The whole point is to know whether your flame becomes cellular (enstrinc instabilities win) or if they get damped and you remain laminar
To do that, asses the sign of

$$\omega_{tot} = \omega_{\textcircled{DL}}\left(1 - \frac{\mathcal{M}}{Pe}\right) = \text{exponential growth of enstab "amplification factor"} = \begin{cases} <0 & \text{STAB} \\ >0 & \text{UNSTAB} \end{cases}$$

(DL: Darrieus-Landau)

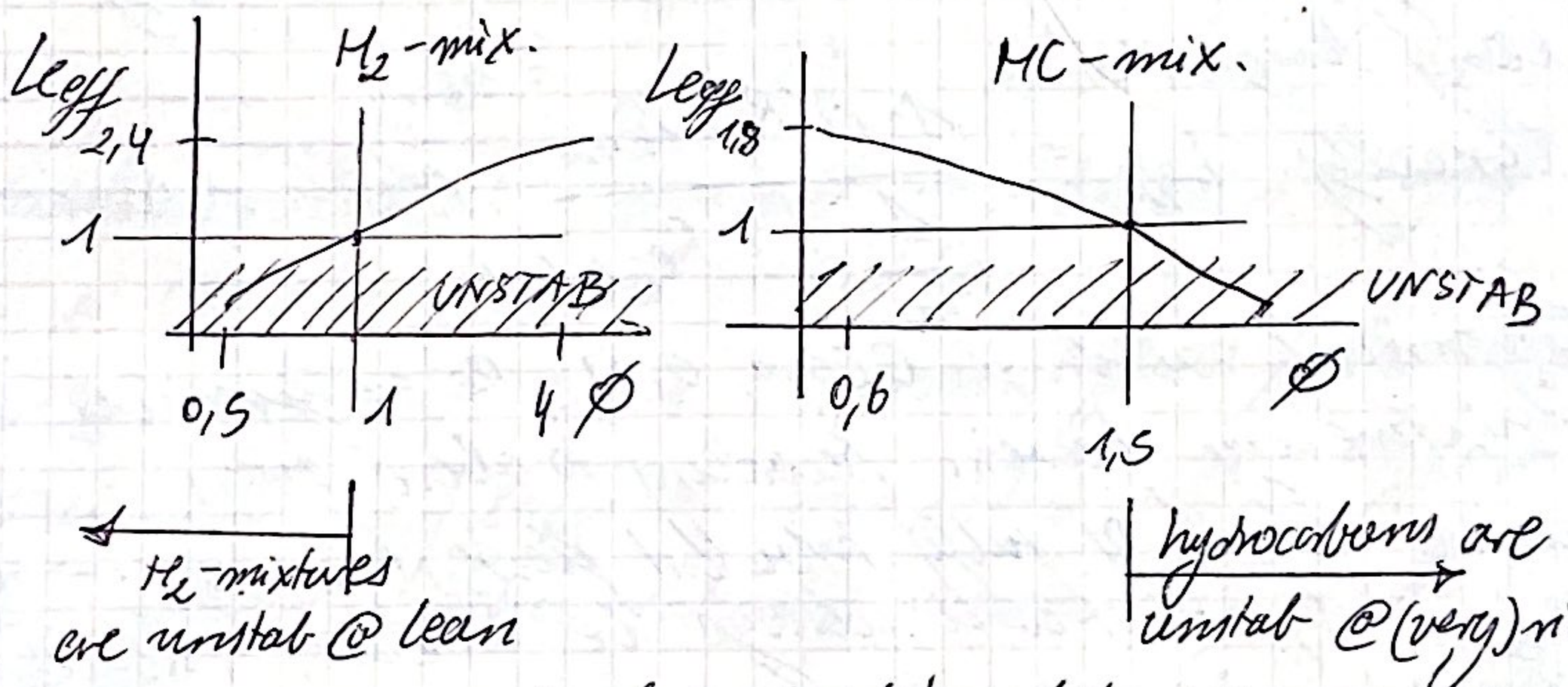
- ω_{DL} = D-L amplification factor due to the hydrostatic enstab. $= f\left(\sigma := \frac{\delta_M}{\delta_b} > 1\right) \propto S_L \cdot K$ always >0!
- $K = \frac{1}{\lambda}$ = wave number; λ = wavelength

• Ri is a highly fucking complicated term (Oppong)

$= f(Le_{eff}; \sigma, Tadiabatic)$

note that $Ri \propto (Le_{eff} - 1)$, so if $Le_{eff} < 1$ or ei more complicated cases / models if $Le_{eff} < Le_{crit}$, (Lecrit = critical Lewis #), then $\omega_{tot} > 0$ so UNSTAB.

Le_{eff} is usually $\in [0,5 ; 1]$ and for most mixtures $Le_{eff} \approx 1$, so not UNSTAB. But for H_2-mixtures Le_{eff} can be as low as 0,8, so you observe instabilities. Further remember this:



So H_2 is unstab for lean (only) while HC-mix's can also become unstab but only for rather rich.

"diffusively" radius of the sphere

• Pe = Péclet # = $\frac{\text{rate of advective transport rate}}{\text{— " — diffusive — " —}} \approx \frac{v_{flame}}{S_L}$ lam. flame thickness

So ei conclusion / observations

• Pe has a role: depends on sign of Ri it can amplify or stabilize

• Ri is determined by Le$_{eff}$ which

rics with fuel type & σ. It also depends on Markstein length (as seen below), so speed of the flame. It dives the stability of the flame by decreasing the sign of $\sigma_{Markstein}$. L_{eff} only slightly below 1 is not enough to cause instability. You need $L_{eff} < L_{crit}$, with $L_{crit} \ll 1$ (like 0,5 or 10)

- Thermal & momentum diffusion always have a stabilizing effect — it's only the mass diffusion that can be destabilizing (dependence on L_{eff})
- Gravity can dampen the disturbances but only @ long timescales.
- Usually $L_{eff} = \dfrac{1 + a\, Re_{turbulent}}{\frac{1}{Le} + a\, Re_{turbulent}}$ which is semi-empirical with $a \in [0,1; 0,2]$, Re = Reynolds, $\overline{Le}$ = mixture avg Lewis. Acordingly to above then in the limit of fully turbulent flow, $Re_{turbulent} \to \infty$, $L_{eff} \to 1$, so it will always be STABLE! Turbulence has a stabilizing effect.
- more $\dot{\omega}_{PL} \propto \sigma$
  $\propto S_L \cdot K$, faster flames or bigger expansion ratios σ (like for H_2) cause amplification of instability, if present. So hydrogen flames quickly become unstable if the threshold is passed.

5. Intermezzo — flame stretch.

Any time a flame surface is forced to grow or deform, every element of that surface sees a stretch rate K. In a spherically expanding bomb it's simply

$$K := \frac{1}{A}\frac{dA}{dt} = or = \frac{2S_L}{R}, \quad S_L = \text{local}$$

burning speed, R = instantaneous radius (consumption speed)

How does the stretch modify the local burning speed?[2]

Markstein noticed that if you plot the measured burning speed S_b against K, you can make a lin. fit:

(only for $Le-1$ small & weakly stretched) K_{small}

$S_b = S_b^0 - K L_b$, L_b is a phenomenological constant — Markstein length. L_b is closely related with Le:

- if $Le < 1$ (mass diffuses faster than heat, e.g. very lean H_2-mix), $L_b < 0$. Negative L_b means stretch actually causes $S_b \uparrow$ as $K \uparrow$. But S_b increases K ($K = 2S_b/R$) and this positive feedback loop is destabilizing
- if $Le > 1 \Rightarrow L_b > 0$, so $K \uparrow \Rightarrow S_b \downarrow$ $\Rightarrow K \uparrow$ & so on until it gets damped to zero (it's like the flame is caught in an elastic wrap that the more stretches the more force it exerts to bring the flame there smaller)

Markstein length is often nondimensionalized to compare easily across many flames:

$$Ma := \text{Markstein \#} := \frac{L_b}{\delta_L}$$

6. Now, as it turns out the

advection term is $\propto$ to $\left(1 - \frac{2Ma}{Pe}\right)$

(apart from the $1 - \frac{\pi}{Pe}$) term.

Oppeng has shown:

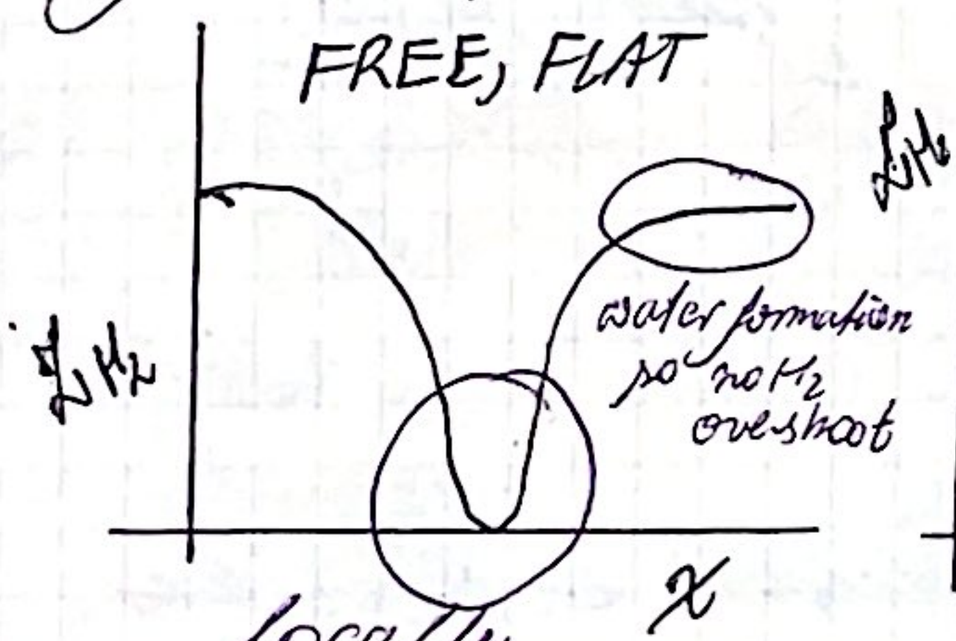
- $Ma > +5$: sketch is so strongly stabilizing that thermo-diffusive (TD) or hydrodynamic instability cells (DL) hardly grow
- $Ma \in [0;5]$: TD still damps short waves, but DL may even destabilize later
- $Ma < 0$: both TD & DL instabs are always reinforced; cellularity starts early & grows fast

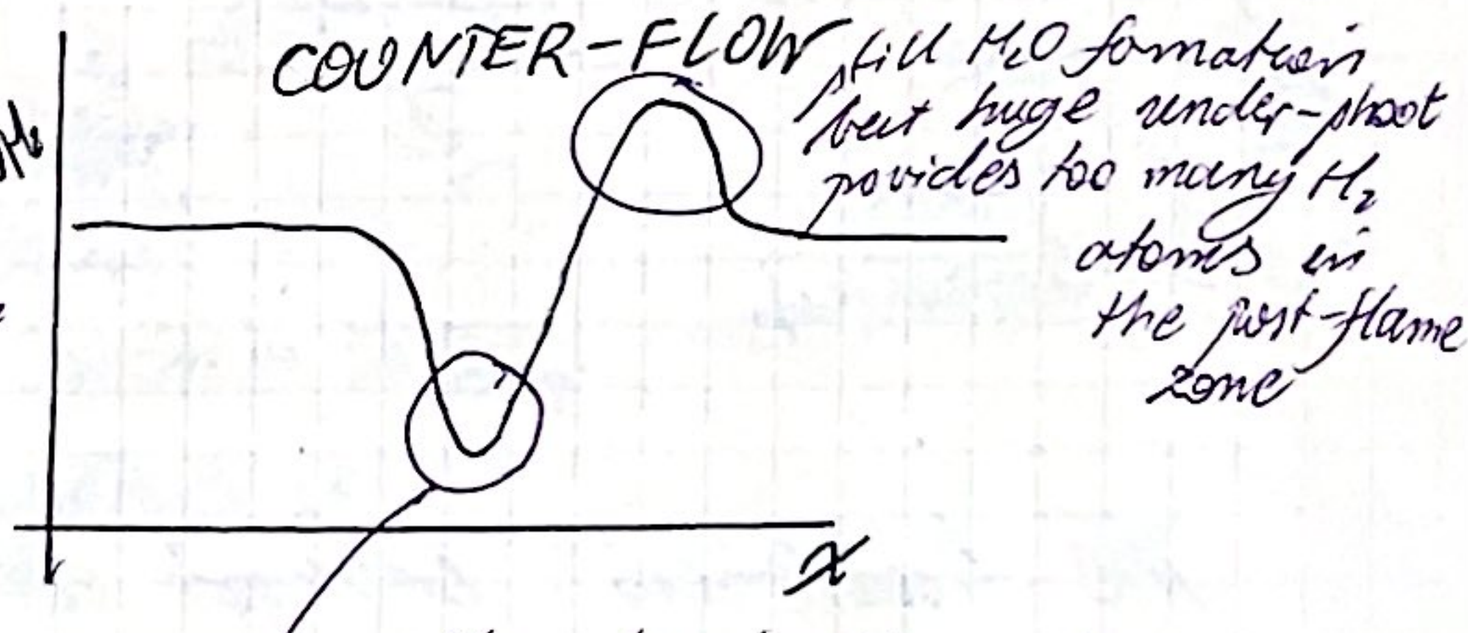
But notice that the "positive-Markstein protection" vanishes in the limit $Pe \to \infty$ or when $v_{flame} \to 0$. So even if flame is stable, the wrinkling may begin if radius is big enough ("small flames are safe").

7. What you also need to consider is differential diffusion — different species have different mass diffusion which changes local equivalence ratios. As a result, the mixture fraction conservation eqn:

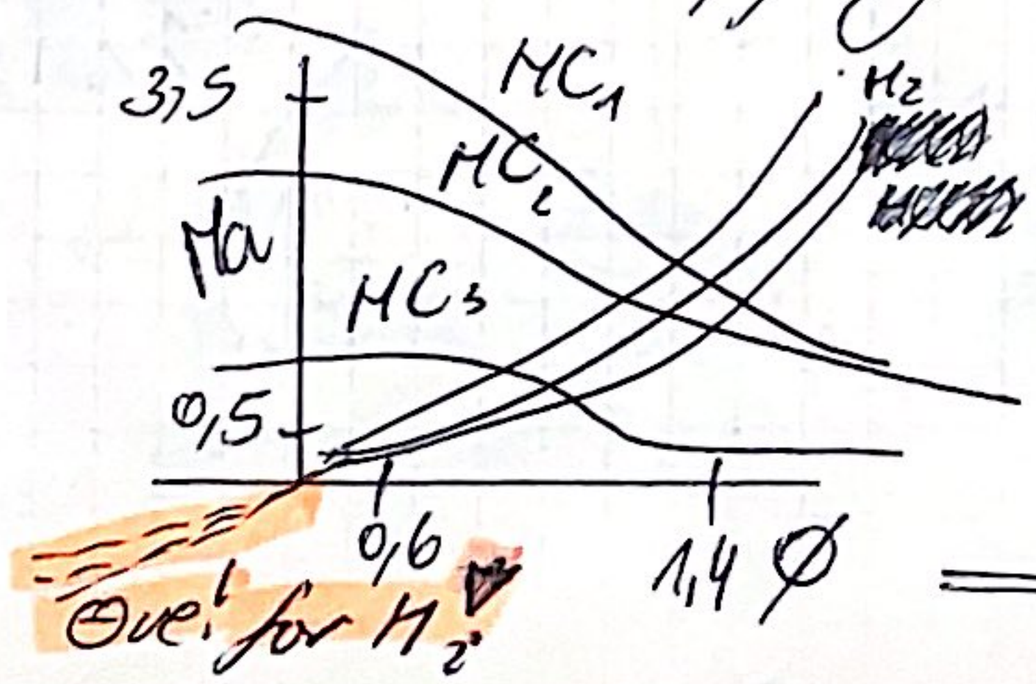
$$\frac{\partial}{\partial t}(\rho Z) + \nabla\cdot(\rho Z \vec{v}) = \nabla\cdot\rho D \nabla Z$$

is no longer true. This is because the assumption for the above is for all species k to have the same diffusivity D_k. For hydrogen this is clearly impossible ($D_{H_2} \approx 20!$). To show the local changes in ϕ consider:





The above & Oppong's Figure:



⟹ leaner mixtures (even locally) have higher tendency to become unstable (Ma ↓); + fuels! ⟹ All be of differential diff!

8. Thermoacoustic instabilities

① A fluctuation in pressure creates a fluctuation in local flame velocity

② The velocity fluctuation affects the flame position & speed, causing a fluctuating HRR

③ The fluctuating HRR can change a velocity of the flame to pressure again.

The dynamic response (forced) can be quantified by **flame transfer fn**:

$$\frac{\dot{Q}'(\omega)}{\bar{\dot{Q}}} = G \cdot e^{\underbrace{+i\varphi(\omega)}_{fn(\omega),\ phase\ lag}} \frac{u'(\omega)}{U_{bulk}}$$

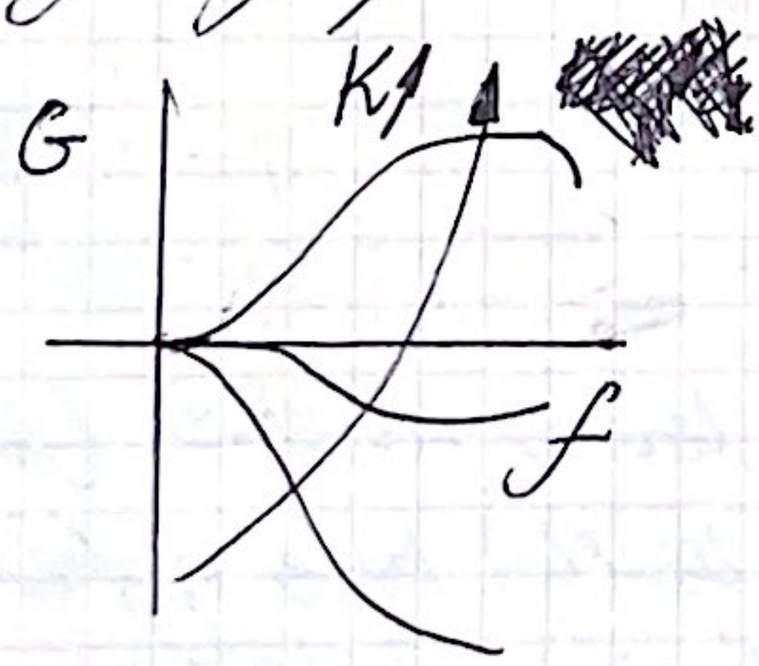
$\dot{Q}$ = HRR

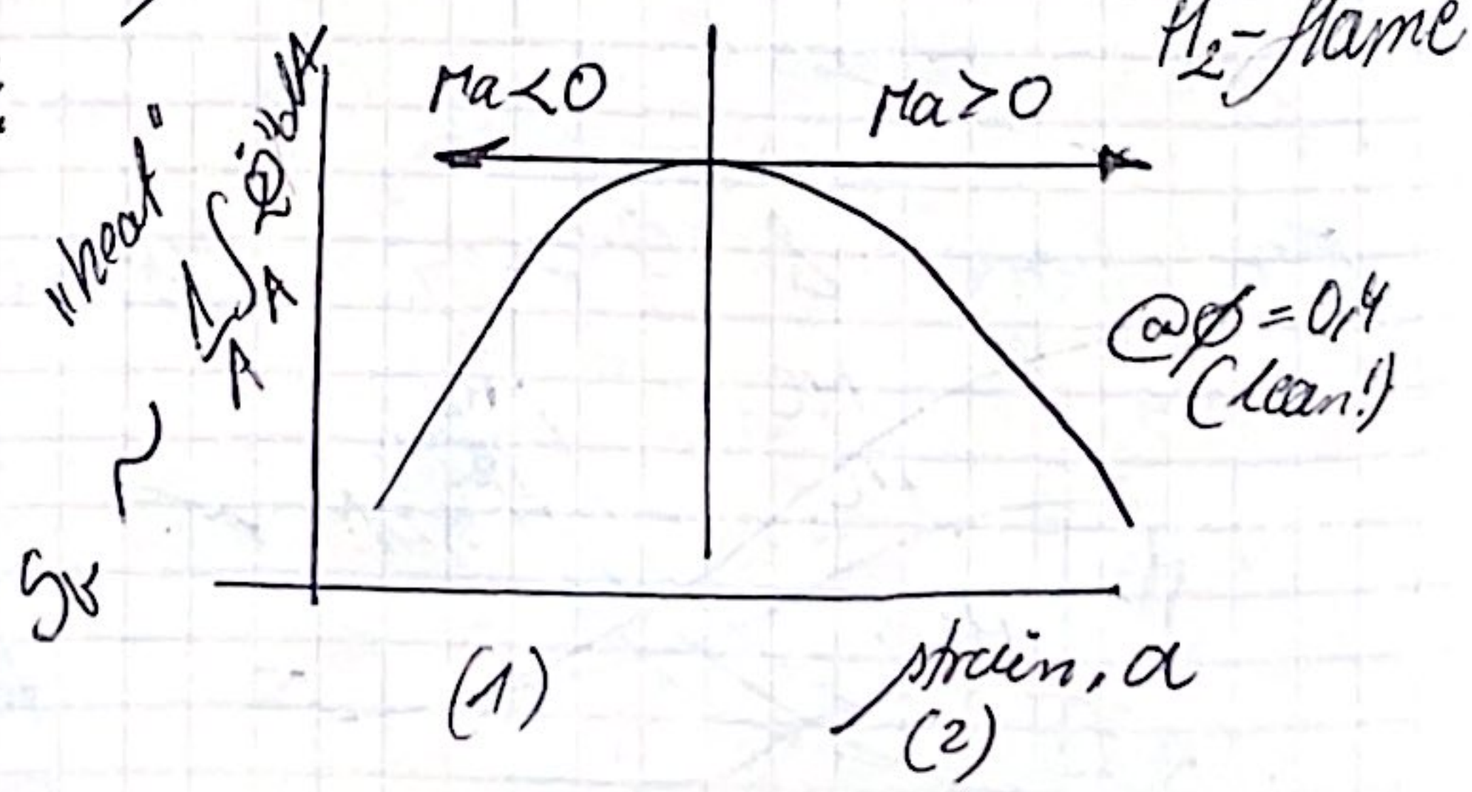
$\bar{\cdot}$ = mean

$\cdot'$ = fluctuation

G = gain

"Built-in" intrinsic cellular instabilities interact with acoustics — if $Ma<0$, they add energy to pressure waves, so a H_2-flame can drive thermo-acoustic oscillations@ for higher frequencies. cmp to HC.





(1) : $Ma < 0$: @ low strain the hydrogen front is only modestly thinned. Extra strain sweeps a little more H_2 into rr-zone than heat can remove, so $\phi \uparrow$, $T \uparrow$, $\frac{1}{A}\int \dot{\omega}'' dA \uparrow$, $S_b \uparrow$, so $\partial S_b / \partial a > 0 \Rightarrow Ma < 0 \Rightarrow$ feeds instability (in phase, ⊕ve loop feedback)

(2) $a \uparrow \Rightarrow \dot{\omega}'' \downarrow \Rightarrow Ma > 0 \Rightarrow$ dampens instabilities. (⊖ve feedback loop).

MC's don't have this issue cuz their $Le_{eff} \simeq 1$ or $Ma > 1$ so always in opposite phase to instability

9. Lean-Jet Technologies for H_2 :

a) Axial air injection

PROS	CONS
– push air downstream so less FB	– increases ΔP_{drop} – affects ϕ

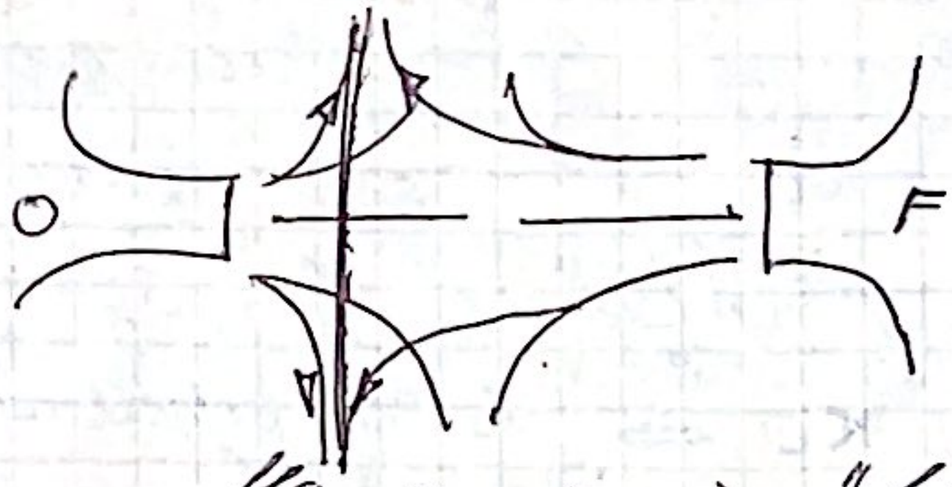
b) Water Injection

PROS	CONS
– reduce temp so NO_x – returns η_{cc}	– lowers η_{th} – need to highly pressurize H_2O

c) Dual Fuel

PROS	CONS
– reduce H_2-storage onboard – control instabilities	– reintroduce carbon – separate & complex pipelines

d) Strain lock



flame → is "locked in place" due to high tangential strain.

PROS
- avoids FB (but only passively)
- reducing NOx (low t_R?)

CONS
- difficult implementation
- unclear instabilities

e) Trapped vortex system with temp. ctrl.



PROS
- reducing NO_x due to lack of O @ rich
- mixing ctrl

CONS
- Unknown instabilities
- unclear limits of low Temp.

(14) Combustion & Turbulence Modeling

1. Starting from the MASS, MOM & EN, these eqns are difficult to solve directly (numerically) (DNS) (heavy). For simplification, apply averaging

$\phi = \bar{\phi} + \phi'$, with $\overline{\phi'} = 0$. $\overline{\bar{\phi}} = \bar{\phi}$. Thus is RANS.

In LES or RANS w/o cc ρ is const so the density terms are not unclosed, may be taken out of the ensemble / SGS filter. But in cc this is not allowed since ρ varies vastly due to HRR. Take for instance GLOBAL MASS:

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho u) = 0 \qquad (*)$$

decompose $\rho = \bar{\rho} + \rho'$ etc & like (*):

$$\frac{\partial}{\partial t}\bar{\rho} + \nabla\cdot\left(\overline{\bar{\rho}\bar{u}} + \overline{\bar{\rho}u'} + \overline{\rho'\bar{u}} + \overline{\rho'u'}\right) = 0$$

($\overline{\bar{\rho}u'} = 0$, $\overline{\rho'\bar{u}} = 0$)

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho u_i} + \overline{\rho' u_i'}\right) = 0$$

But the term $\overline{\rho' u_i'}$ is unclosed (unknown), & if not treated differently must be modeled. To avoid such complications, use a FAVRE filter to solve the closure problem:

$\phi = \tilde{\phi} + \phi''$: $\tilde{\phi} := \frac{\overline{\rho\phi}}{\bar{\rho}}$, $\tilde{\phi''} = 0$.

notice how by this defn : $\overline{\rho''\phi''} = \overline{\rho''\cdot\phi''} = 0$ ← RANS filter ($\rho'' \to 0$)

and $\overline{\rho\phi} = \hat{\phi}\bar{\rho}$. So no more unclosed terms of form $\overline{\rho' u_i'}$. Then (*):

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\right) = 0$$, which is by the way identical to RANS-averaged MASS with ρ = const.

The above ("Reynolds-averaging-outcome") is true $\forall$ MASS, MOM, EN.

Avg momentum. RST, unresolved, must be modeled

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_j) + \frac{\partial \bar{\rho} u_i'' u_j''}{\partial x_i} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_j} - \frac{\partial \bar{\tau}_{ij}}{\partial x_i} + g_i$$

Avg energy turbulent energy-flux, also unclosed

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{e}\tilde{u}_j) = -\frac{\partial}{\partial x_j}(\overline{\rho e'' u_j''}) - \frac{\partial}{\partial x_j}(j_{cond} + j_{int-diff})$$

So FAVRE apart from generating classical RST & turbulent energy-flux terms, has one BIG disadvantage: the reaction rate $\overline{\dot{\omega}_i}$ is also unclosed: This is because

$$\overline{\dot{\omega}_j} \neq A_j \cdot \tilde{T}^{\beta_j} \exp\{-E_a/R_0\tilde{T}\}[\tilde{X}_A][\tilde{X}_B] !$$

('cuz Arrenius is highly nonlinear!)

(Note: we're talking here about local species MASS:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_k) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{Y}_k) = \frac{\partial}{\partial x_i}\left(\bar{\rho}(D_{turbulent} + D_k^M)\frac{\partial \tilde{Y}_k}{\partial x_i}\right) + \overline{\dot{\omega}_k}$$

If the inequality above is assumed to be true, then it "underestimates peak concentrations" IL.

Note the RR issue is independent of the "mesh filter, i.e. if it's Raynolds or Smagorinsky.

"Is FAVRE equally suitable for premixed & nonpremixed"

2. Some Modeling Approaches

A) General:

a) Eddy Breakup (crude)

b) PDF / FDF method (expensive)

B) Non-premixed approaches

c) mixture-fraction method

d) conditional moment closure

C) Premixed approaches

e) Flame surface density

f) Flamelet / progress variable methods.

~~a) Eddy breakup method~~

3. LES → resolves: explicitly compute large scales while model subgrid scales (small ones).

When applying ⍉, the turbulent terms are SGS stresses, SGS scalar fluxes, and $\dot{\omega}$ → for SMAG. FILTER $\overline{\dot{\omega}}$: SGS filtered reaction rate. All q-ties Q are subject to a cut-off filter: $\overline{Q} = \int Q(\xi) F(x-\xi) d\xi$ & $\overline{\overline{Q}} \neq \overline{Q}$ (unlike RANS)
↳ res. filter

a) Eddy Breakup Model:

chemistry is ∞-fast ("mixed = burnt")

replace the chemical source term with a "mixing-limited" term $\overline{\dot{\omega}_k} = -C_{EBU} \overline{\rho} \frac{\varepsilon}{k} \overline{Y_k}(1-\overline{Y_k})$

VERY CHEAP but CAN'T CAPTURE CHEM. KINETICS.

since chemistry is ∞-fast

that in practice means you bypass any chemical q-tities, just make $\dot{\omega}$ depend on concentrations (mixing)

b) Transported PDF method (PDF/FDF)

PDF = probability density fn. ↑ "Subgrid PDF"

FDF = filter density function

we define the filter PDF/FDF

$$\overline{\dot{\omega}_k}(x,t) = \int \dot{\omega}_k(\psi) \widetilde{P}(\psi; x,t)\, d\psi$$

ψ some quantity (actually I think ALL qtties)

So basically you reject the ∞-fast chemistry (Exact Arrhenius) in favor of modelling the RR stochastically: you filter RR with unknown FDF (joint) depending on all thermochemical variables $\psi = (T, P, Y, \ldots)$. If you knew $\widetilde{P}$, chemistry rate $\dot{\omega}_k(x,t)$ would be exact. Problem is you don't know $\widetilde{P}$. You can write transport eqn for that but because of the diffusion term ("transported PDF") you can't solve it. You must solve for the term: $\int \omega P\, d\psi$ (+ very expensive, sometimes even more than DNS) using other methods — Monte Carlo (Pope). Inject particles & track them using Lagrangian frame. You assume the particles move according to a velocity that has both stochastic (turbulence) & deterministic form. When you track them you can predict flow properties (eg: ?).

The advantage is now that for each separate particle reaction rate is a closed term but

the effect of micromixing must be employed, as it depends on all other particles around.

We're doing all this because solving the transport for PDF / FDF is not beneficial.
~~Instead we inject "artificial" / notional particles representing fluid samples~~. The FDF lives in a space whose dimensionality = number of scalas {Y} + dim x + dim t. ~~So~~ Pope's

many! 3 1

So solving numerically a PDE in ≈25 dimensions is impossible!

Monte Carlo circumvents this absurdity by injecting thousands "Notion Particles" in Lagrangian frame. Each ~~velocity of the~~ particle has a det. velocity plus a stochastic fluctuation (Brownian), that mimics turbulence. Then you can easily integrate your time ODE's provided you obtain some simple mixing model. But there's a price — you need 20-50 particles per cell to keep the sampling error small, else the averaged quantities which are the result of this Monte-Carlo become noisy & unstable.

To make this more affordable for LES or realistic combustors, the "stochastic-fields" variant abandons Lagrangian tracking & instead solves 4-8 "component fields", each driven by an independent random forcing. Chemistry is still integrated exactly but memory requirements are greatly reduced.

Whether you use M-C or Wolfastic fields the logic is the same: keep entier Arrhenius, model only the small-scale micromixing and recover the source as terms by averaging over the ensemble. That makes the transported PDF the most accurate turbulence-chemistry closure short of DNS. Problems are: heavy & residual dependence on how you model micromixing. But wherever finite-rate chemistry matters, no cheaper model can match it's fidelity.

4. You can also use the "artificially thickened flame methods". (ATF)

→ If you're using LES, then it's impossible to correctly capture $\dot{\omega}_k$, since a real flame is only a couple ~~mm~~ μm thick, so any realistic LES filter will always cut it off.

Solution? Instead of $\Delta \to 0$ (DNS), inflate the flame: multiply diffusivities with factor F which spreads the temp & species gradients over F times the natural width. At the same time, every Arrhenius RR is divided by F to keep correct flame speed. This thickening of the flame, however, erases the small wrinkles that turbulence would've engraved, so ATF introduces an algebraic

efficiency E_{TURB} that boosts the source term wherever SG turbulence is strong restoring the right turbulent flame speed:

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i}\left(\rho \cdot E_T \cdot F \cdot \frac{\partial Y_k}{\partial x_i}\right) \cdot \frac{E}{F}\dot{\omega}_k$$

(E/F: correct turb speed (wrinkling); E: correct lamin speed (thickening))

5. Everything above so far explains many transport eqns currently encodes the computational effort significantly. Two types of methods to deal with it:

1) use skeletal mechanisms
(i.e. remove unimportant species)

2) Geometrical or statistical approaches.

6. Flame Surface Density Methods (FSD)

Visualize the flame as a brush separating reactants & products. To describe "how tightly the bristles are packed" use Σ: flame-surface density. FSD You can write transport for Σ → inexpensive cuz it doesn't contain any chemistry, S_L is a "material property" known. Then RR follows as $\dot{\omega} = \rho S_L \Sigma$. The required by LES SG turbulent flame speed $S_{T,\Delta}$ is then immediately retrieved:

$$S_{T,\Delta} = \frac{\rho S_L \Sigma}{\rho u}.$$

However, often, with less computations you can resolve the flame speed $S_{T,\Delta}$ directly from transport equations for c.!

$$S\left(\frac{\partial}{\partial t} + \bar{v}\cdot\bar{\nabla}\right)c = s_u S_{DNS}\,|\bar{\nabla}c| \qquad (DNS)$$

$$S\left(\frac{\partial}{\partial t} + \bar{v}\cdot\bar{\nabla}\right)\bar{C} = s_u S_T\,|\bar{\nabla}\bar{C}| + \dots \qquad (RANS)$$

$$S\left(\frac{\partial}{\partial t} + \bar{v}\cdot\bar{\nabla}\right)\tilde{C} = s_u S_{T,\Delta}\,|\bar{\nabla}c| + \dots \qquad (LES)$$

and there is a relation

$$S_{DNS} < S_{T,\Delta} < S_T$$

Note that the following checks should hold

- $\forall$ grids $\lim_{\Delta_{grid}\to 0}(S_T) = S_T$, grid independent (convergence)
- $\lim_{\Delta\to 0}(S_{T,\Delta}) = S_{DNS}$ (consistency)

7. "The Flamelet assumption" (FM = flamelet model(s))
If local Karlovitz # is small, the turbulence only wrinkles / folds the flame s/o changing the internal structure (homomorphic). Because the 1-D ~~flame~~ laminar flame is pre-computed every thermodynamical quantity — temp, ρ, ω — can be tabulated as a fn of 1 or 2 control variables — prem: c (progress var); diff: Z (Bilger mixture fraction. In any case the source term is always available as it's only of 1 variable (c or Z). But only holds for $Ka < 1$!

Note that in case of nonpremixed, the "lookup table" has to be parametrized not only with Bowgh mixing fraction but also with scalar dissipation rate:

$$\chi = 2D_k(\nabla Z)^2. \quad (\text{OR STRAIN})$$

So to summarize: Flamelet assumption lies in the middle between expensive & accurate transport PDF method and crude eddy breakup method — that's why it's preferred in the industry.

& With the flamelet assumption, you still might encounter that your cell size is bigger than δ_L. In that case you can use the "artificially thickened flame method" or do the following: "Presumed PDF approach" RR, or any thermochemical q-tity can be averaged using a presumed PDF

$$\rightarrow A\delta(c^*) + \frac{B}{|\nabla c^*|} + C\delta(1-c^*)$$

$$\overline{\mathcal{Q}} = \int_0^1 \mathcal{Q}(c) \cdot P(c^*; \underbrace{E[c]}_{\tilde{c}}, \underbrace{Var[c]}_{\tilde{c''^2}})\, dc^*$$

For this to be precise, you usually require second order accuracy $P = P(E[c]; Var[c])$

it's stochastic analogue of turbulence (randomness)

In case of nonpremixed P is also a fn of $E[Z]$, additionally. $Var[Z]$ is not necessary because

you can write transport for it

$$\bar{s}\frac{\partial \widetilde{Z''^2}}{\partial t} + \bar{s}\tilde{u}\cdot\nabla\widetilde{Z''^2} = \cdots - 2\bar{s}\bar{\chi}$$

↑ SDR

where $\widetilde{Z''^2} = Var[Z]$. Notably $\bar{\chi}$ is unclosed but a transport model exists for it which closes it. So χ is the sink for transport of $\widetilde{Z''^2} = Var[Z]$.

With the presumed PDF dependent only on c (pres.) and Z (in case non-pres), which in turn depends on χ which is closed by its own transport eqn, one has

$$\overline{\dot{\omega}} = \int_0^1 \int \overline{\dot{\omega}(c,z)}\, P(c,z, E[c], Var[c], E[Z])\, dz$$

(or: nonpremix) to depends on ξ (c and Z), and can be plugged into transport of c into LES variant (see earlier)

3. Now, obvious limitations of the flamelet model it's ignore assumption: turbulence doesn't effect chemistry, which is not always true. Also the presumed PDF approach assumes no fast chemistry, so the model will struggle with slow effects such as NO_x or CO. Can be take it better if you include covariance.

"mixed is burned"

10. The NO_x modell. & FM

To allow the presumed PDF approach (which assumes ∞-fast chemistry) to account for slower processes like NO_x formation, the simple fix is to solve simultaneously transport of C AND of NO_x:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_{NO_x}) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{Y}_{NO_x}) = -\frac{\partial}{\partial x_i}\bar{J}_{NO_x} - \frac{\partial}{\partial x_i}(\overline{\rho u_i'' Y_{NO_x}''})$$

If this method takes into account the "residence time"

11. Partially Premixed Flamelets: Flamelet Generated Manifold (FGM) & FM

using e.g. the presumed PDF approach

Flamelet models were ~~generated~~ formulated first separately for premixed & non premixed. For partialy premixed we need a description in terms of both mixture fractions & progress variable. Since now you need $\tilde{E}$ & $\widetilde{Var}$ for both C & Z, your table beomes multidimensional (4-5 dimensions), to cumbesome

↳ with covariance

12. Modeling of Hydrogen flames

a) Suppose the mesh size $< \delta_L \Rightarrow$ the TD instability is captured as long as you predict correct flame speed. For small curvatures, including diff-diff only inside the flamelet might be enough. Otherwise, you need 2D parametrization (2D flamelets)

for FM methods:

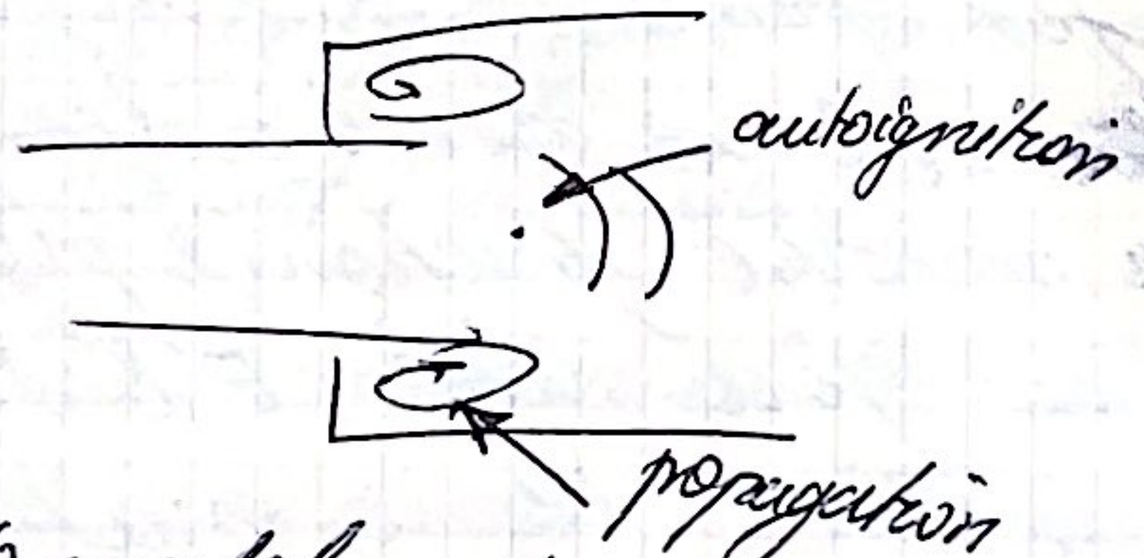
b) If mesh size is larger than the laminar flame thickness → the surface growth rate of the TD instability needs to be modeled (reaction rate):

$$\omega_{tot} = \omega_{DL}(1 - \mathcal{K}/Re) = f(K)$$

(only need to model $\mathcal{K}$ when $K <$ mesh size

For a FM the PDF might depend on further params.

c) autoignition — depends strongly on chemistry so the choice of model for ω is very relevant. ~~You need~~ In case of hydrogen you need to account for autoignition due to the low autoignition delay times.



Need to model the RR: $\omega_{tot} = A \cdot \omega_{prop} + \omega_{autoign} \cdot B$ (Levi condensation). For FM you also need an index to distinguish between autoign & prop regimes.

⑨ Laminar & Turbulent Flames II

1. Temp eqn

$$\underbrace{\rho c_p \frac{DT}{Dt}}_{\text{unsteady convective storage}} = \underbrace{\nabla \cdot \lambda \nabla T}_{\text{heat conduction}} + \overbrace{\sum_{k=1}^{N} \left(\frac{\rho \alpha c_{pk}}{Le_k} \nabla T \cdot \nabla Y_k \right)}^{\text{enthalpy carried by spec. diffusion}} - \underbrace{\sum_{k=1}^{} (\dot{\omega}_k h_k)}_{\text{chemical heat source / sink}} + \underbrace{Se}_{\text{other sources / sinks like radiation, Lagr.}}$$

2. Progress variable

$$c = \frac{Y_k - Y_{k,u}}{Y_{k,b} - Y_{k,u}}$$

if $Le_k = 1 \Rightarrow$ it's equivalent

or $\Theta = \frac{T - T_u}{T_b - T_u}$

Felix not use fuel for the defenition for c cuz denom may vanish (+ diff. diffusion as in the assignment, not monotonic).

c is 0 in reactants & 1 in products. in between must be smooth

3. Thicknesses

$\delta^2 = \frac{\alpha}{S_L}$ stretched (2) laminar flame speed

stretched (2) flame thickness

thermal thickness: $\frac{T_b - T_u}{|\partial T / \partial x|_{max}} = \delta_L^0$

x

4. Speeds

absolute speed : $\frac{\frac{\partial c}{\partial t}}{|\nabla c|} = S_a$ (external observer)

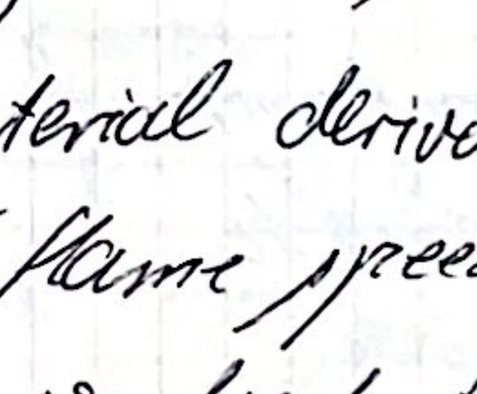
displ speed : $\frac{\frac{Dc}{Dt}}{|\nabla c|} = S_d$ (moving with the flame, difficult to compute)

consumption speed :

$$S_c = -\frac{1}{S_u (Y_{f,u} - Y_{f,b})} \int_{-\infty}^{\infty} \dot{\omega}_{fuel} \, dX$$

= "amount of fuel integrated across the flame per unit of time".

5. Sketch = curvature v strain



6. Denote v = fluid ~~velocity~~ velocity in stationary frame

w = flame velocity in stationary frame

$n \cdot (w - v) = S_d$ = displacement speed : flame speed wrt fresh oncoming reactants

Can show that the material derivative of the progress variable with w (flame speed) is zero (c is conserved along w but that makes sense cuz it's almost defined that way — to show the direction of the rn/flame)

$$\frac{\partial c}{\partial t} + w \cdot \nabla c = 0.$$

↳ we're tracking the flame with c which moves @ speed w so obv $\frac{Dc}{Dt} = 0$.

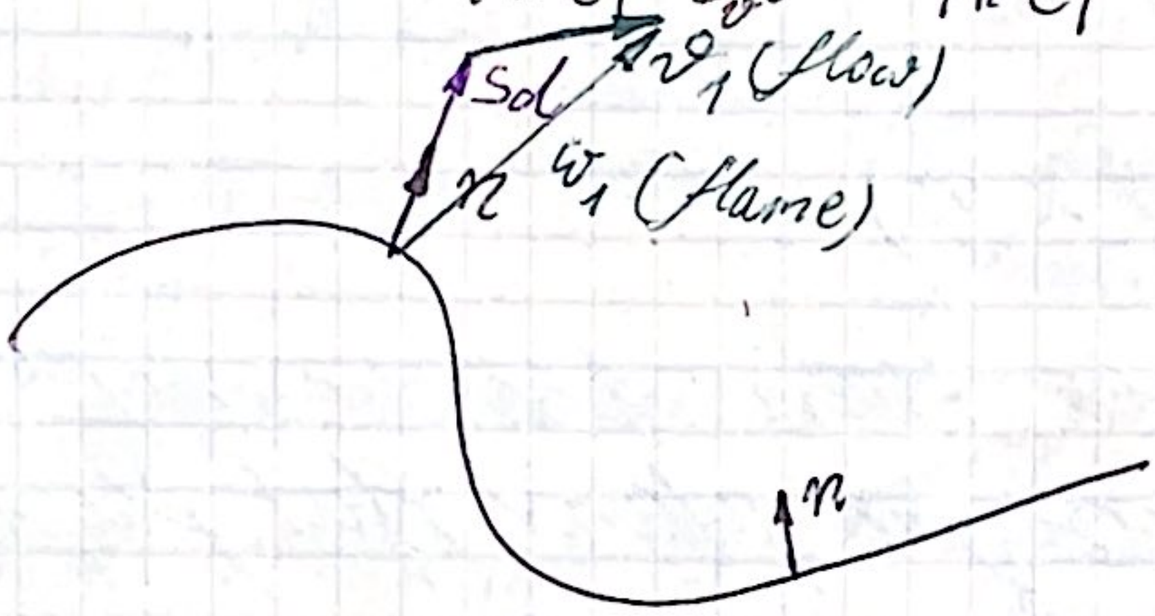
On the other hand, c can change along velocity of the flow, or: if $\omega \not\perp v$, then

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla\right) c \neq 0$$ (this is also seen

from the fact that $S_d = n \cdot (w - v)$)

One can show

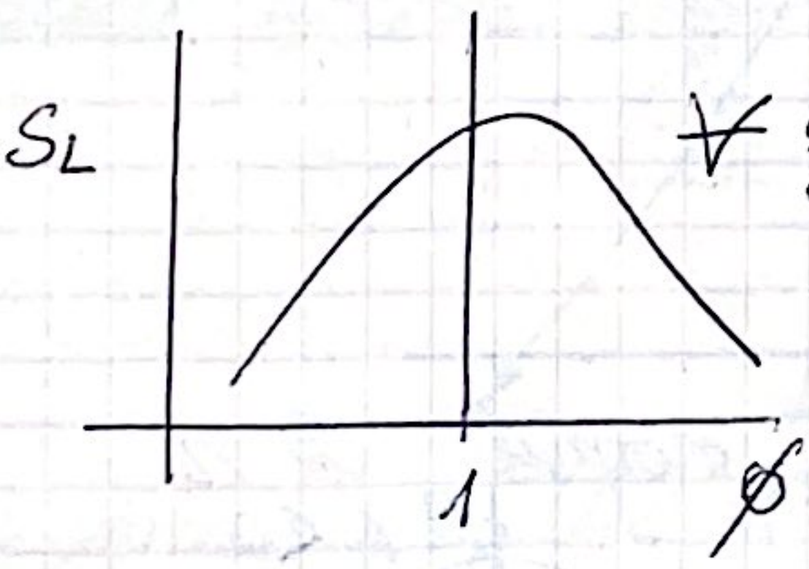
$$S_d = \frac{1}{|\nabla c|} \frac{D_v c}{D t} = \frac{1}{|\nabla c|} \left(\frac{\partial}{\partial t} + v \cdot \nabla\right) c$$



Furthermore, there is a transport for c:

$$\underbrace{S \frac{\partial c}{\partial t} + S v \cdot \nabla c}_{|\nabla c| \cdot S \cdot S_d} = \underbrace{-\nabla \cdot j_m}_{\text{laminar diffusion flux}} + \omega, \text{ so}$$

$$S_d = \frac{1}{S|\nabla c|} \left(-\nabla \cdot j_m + \omega\right)$$

7. 

$\forall \approx$ fuels

Laminar flame speed

$$S_L^0 \propto \sqrt{\frac{\alpha}{\tau_{chem}}}$$

($\tau_{chem} = \frac{\delta_L}{S_L^0}$ so how does it make sense?)

8. Stretch rate K:

$$K := \frac{d}{dt} \ln A = \frac{1}{A} \frac{dA}{dt} = \nabla_t \cdot w_t + (w \cdot n)(\nabla \cdot n)\Big]_S$$

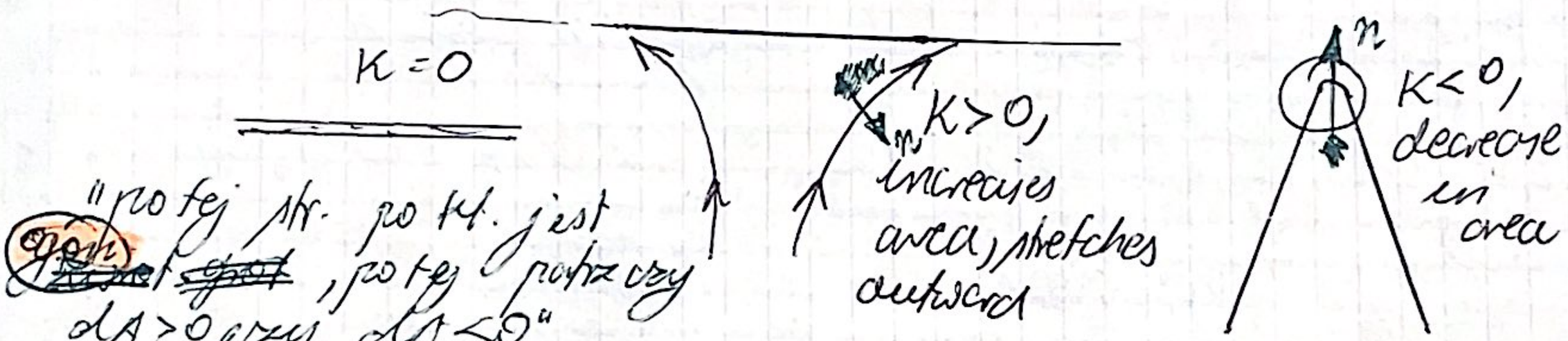
where s is any isosurface (T, C), ..., any isosurface that best marks the flame).

Note stretch has three components:

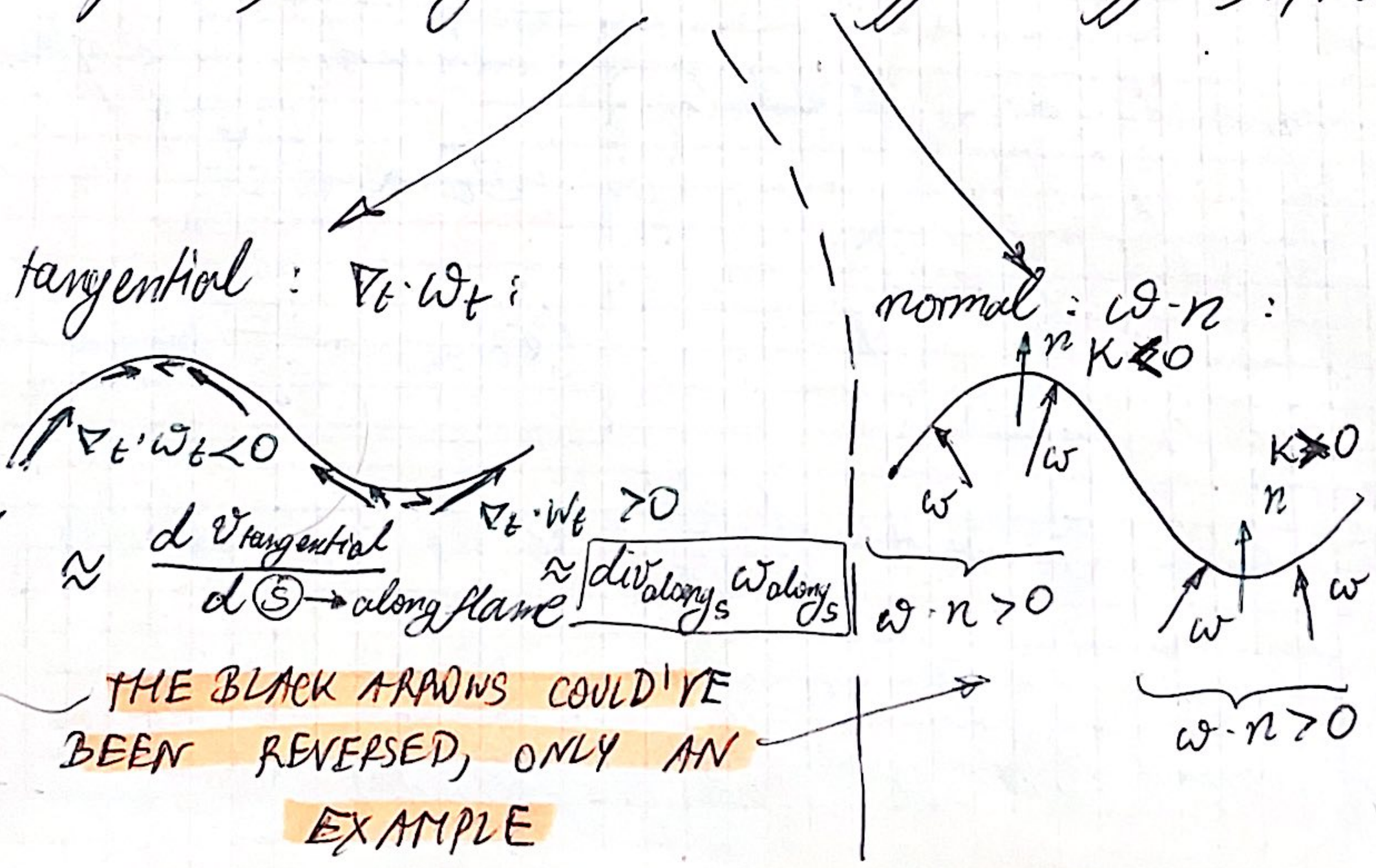
- $\nabla_t \cdot w_t$ = tangential strain, comes from velocity gradients along the surface
- $w \cdot n$ = normal motion (strain)
- $\nabla \cdot n$ = mean curvature

$$= -n \cdot \nabla \times (v \times n)$$

note if n = const then all the components vanish so $K = 0$ for planar flat flame



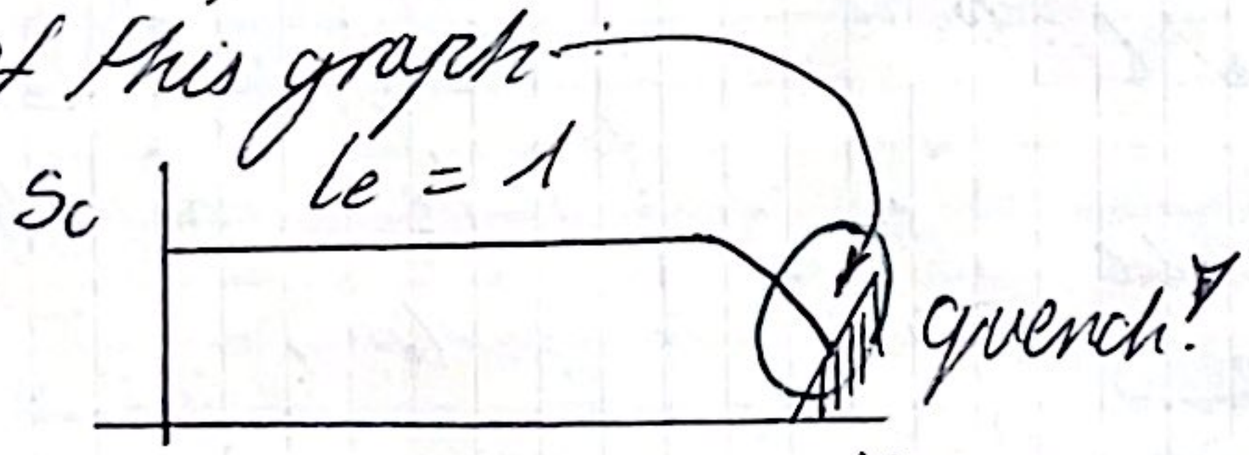
The most important are tangential & normal components. They all have different effects/roles



- tang strain elongates/ shrinks tangentially the isosurface.

- it can thin / thicken the preheat zone. Thus, it affects normal gradients of T, Yk, and so consequently the mass burning rate ω̇.

- Since it affects the gradients & thickness, it also affects residence time. High tang. strain will thin the flame preheat zone so much, it doesn't keep up with the newly oncoming fresh & cold reactants — chemical time / residence time is no longer able to sustain combustion. This is the essence of this graph:



The strain in the circled region is so high, the flame gets quenched! (If you assume all that stretch is tangential strain) Chemical / Residence time is lowered so much / the preheat zone is so thin that it doesn't allow for complete combustion anymore. → extinguish!

- normal strain can move / push the flame ⊥ to it's surface

- so it's role is to move the iso-surface / flame into the region / position where normal flame speed matches the local reactants flow (premixed) (A)

LAW: "Conflicting (opposing) explanations in literature, this is the Kilmov & Williams".

* normal strain!

preheat zone

note: * = this is also why the lock-down technique lowers NO_x! because opposing jet configs provided large tangential strain which in turn lowers t_R, no less yellowish!

Based on the way tangential strain can affect the mass burning rate, we distinguish two cases:

Hydrodynamic Flame (stretch)

- ∞-thin, diffusion is not important
- Flame already ∞thin so no thinning possible by $\nabla_t \cdot w_t$.
- So $\dot{m}$ cannot be modified (mass burning rate = const) $\dot{m}$
- but tang. strain still may tangentially elongate the surface, so that volumetric $\dot{m}/A$ burning rate is increased. (for $\oplus$ve $\nabla_t \cdot w_t$).

Flame Stretch

- here, flame is not ∞thin and does have thickness.
- changing thickness by tang. strain leads to changed mass burning rate (thru changing $\perp$ gradient, T, Y_k profiles).
  this also changes the completeness of the reaction

if $Le > 1 \Rightarrow \dot{m} \downarrow$,
$Le < 1 \Rightarrow \dot{m} \uparrow$

1D normal strain i.e. (⁂):

- if flame is not restrained, then normal stretch is not active / effective: it's only job is to move back & forth to match reactants speed, i.e, to "run away" from the stretch. ONLY if flame is restrained does the normal strain cause preheat zone compression / thinning & in that case, the effect is the same as the tangential strain ⟶ tk ↓, can extinguish the flame eventually.

~~But why does thinning preheat zone actually can cause quench?~~

Back to Hydrodynamic & Flame Stretch.

Hydro

- is governed by Ka
- Can be shown:

$$Ka = K \cdot \frac{\delta_L^0}{S_L^0}$$

- Ka measures when the turbulence or strain start affecting the internal structure of the flame (chemo.)
- The bigger stretch (K), the bigger Ka — makes sense: The same is observed on Borghi: bigger stretch [turbulence], the

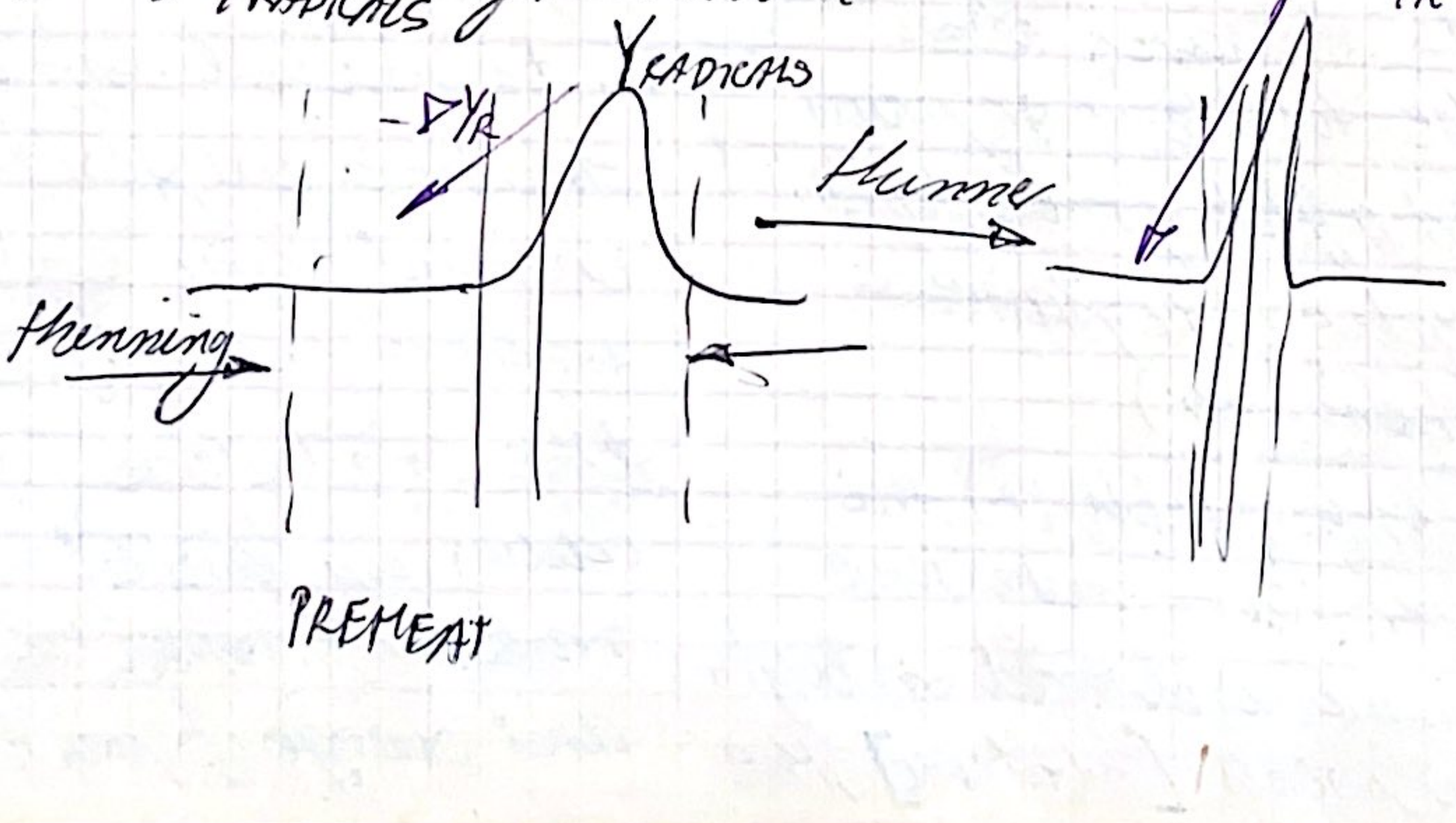
Flame

- is governed by Da
- in stretch context, flame stretch allows for thinning the flame, so altering ∇, t_R, radical diffusion. The above changes the chemical time and flame internal structure, just like in turbulence "all eddies can embed in the rz zone / preheat zone & and change its structure".

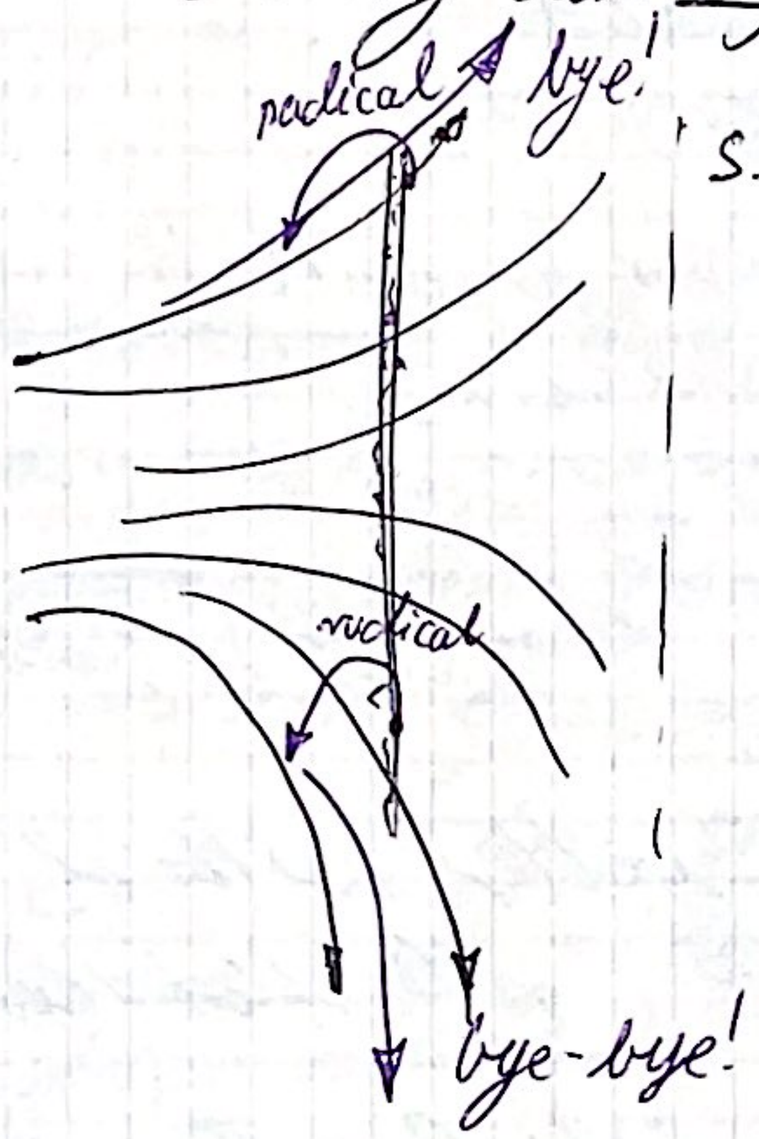
bigger the area of flamelet
[bigger wrinkles by turbulence],
so if keep increasing k_a [$2u'$],
@ some point you will
start changing the internal
structure of the flamelet.

In any case $Ka_2 1$ means
turbulence only wrinkles
flamelet. This is "equivalent"
to stress only ~~tangent~~
tangentially ~~the~~ pulling
out the flamelet ~~to~~
(without the possibility
to ~~ex~~tinguish/quench,
or unaffected, only
~~in~~/A affected)

Intermezzo: Why stirring of the preheatzone can cause quench? If thinner, then steeper $\nabla Y_{RADICALS}$ gradient:



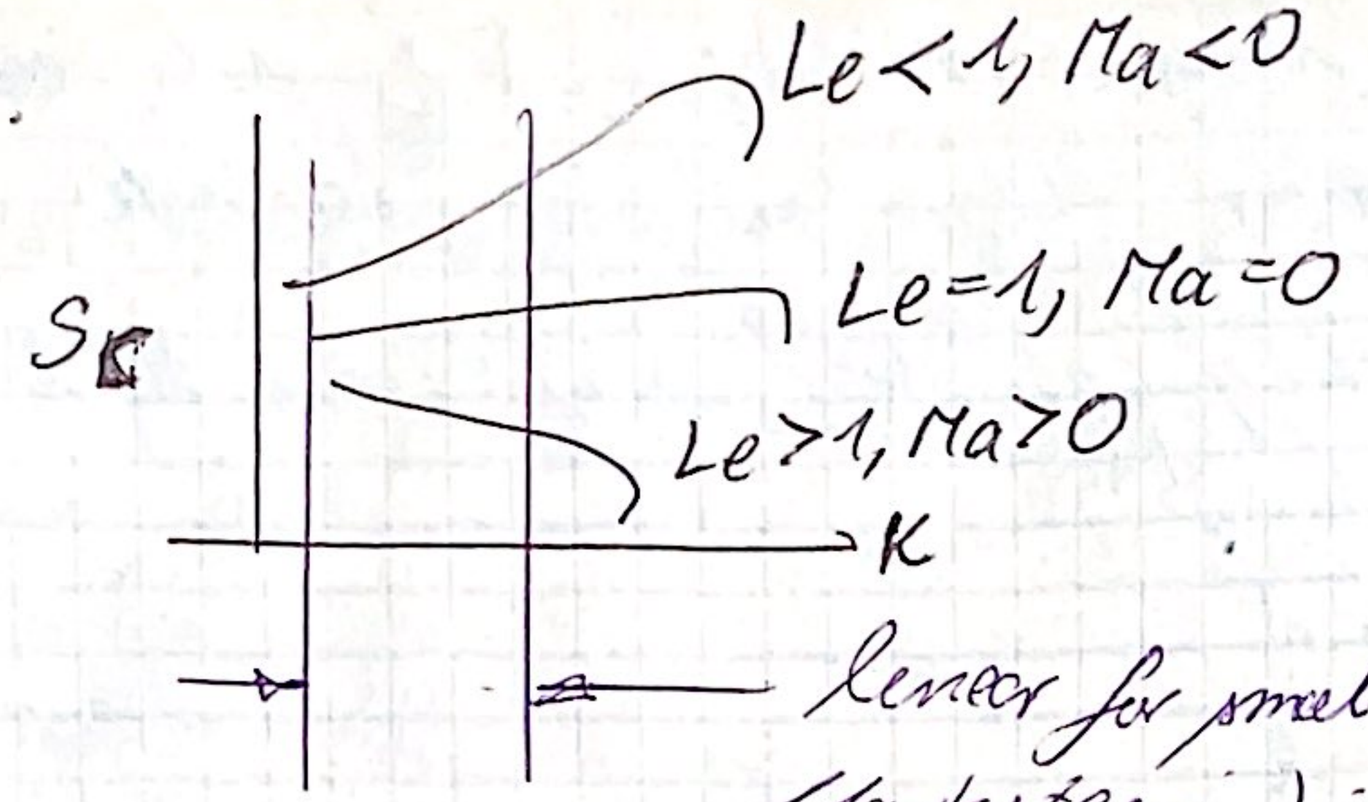
so thinner causes steeper radical ∇Y gradient meaning they're more prone to diffuse back to reactants where they can diff away with incoming reactants



no radicals = unsustained chain reaction!
Also, thin zone means heat is lost, too (it can't explain why), so lower E_a & again can't sustain rxn.

that's why an adiabatic; $Le = 1$; unstretched flame is almost always immune to quench!
(adiabatic = E_a is not lost, unstretched = cannot thin the flame, $Le = 1 \Rightarrow$ heat diffuses @ same rate as molecules).

9.



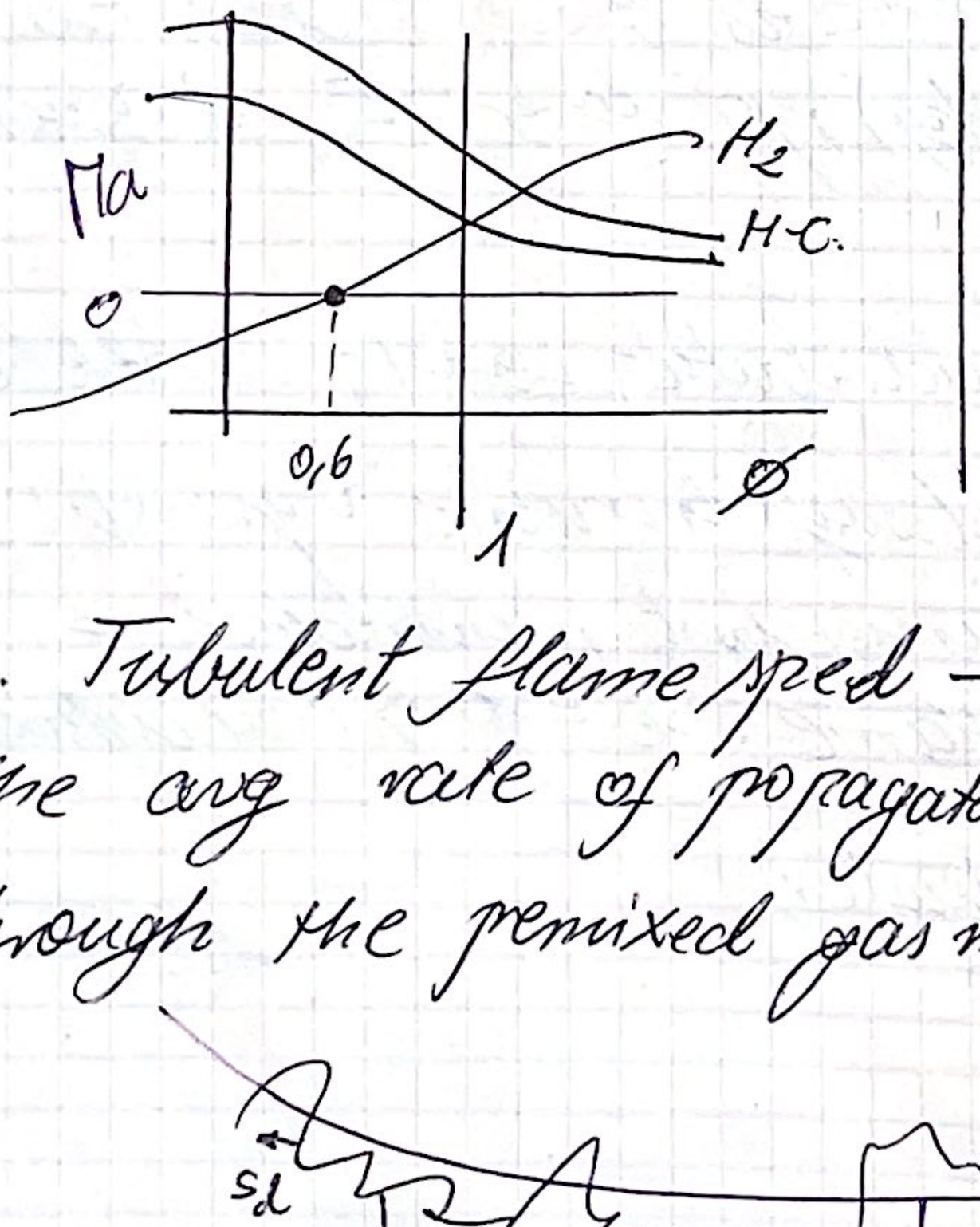
$$Ma := \frac{\mathcal{L}}{\delta_L}$$

linear for small K: (due to Markstein):

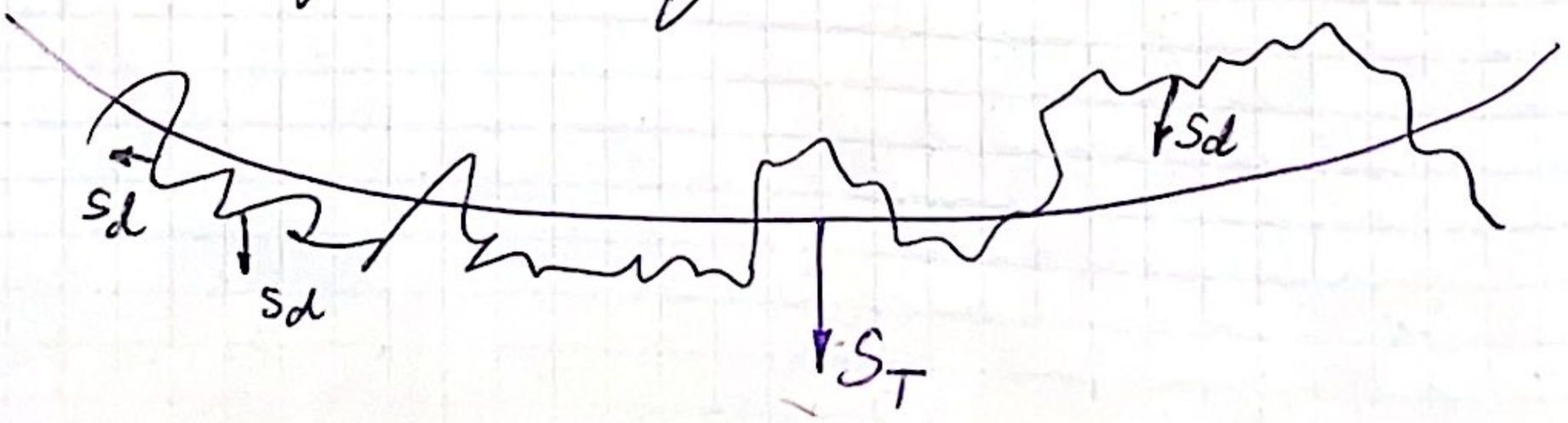
$$S_c = S_c^0 - \mathcal{L} K$$

↳ (1st) Markstein length.

Note: the graph above can be represented better with 2nd order polynomials en $\mathcal{L}$ (nth Markstein lengths?) It's just a model valid for small K & small Le (approx).



eg. Turbulent flame speed — is defined as the avg rate of propagation of the flame through the premixed gas mixture



• The consumption / burning speed is defined the same way as for laminar

$$S_{c,T} = \frac{-1}{A \rho_u Y_{f,u}} \int_{-\infty}^{\infty} \dot{\omega}_f \, dx.$$

• For hydrodynamic flames (or $Ka < 1$, or flamelet assumption, or mixed is burned, or turbulence doesn't affect chemistry, or ∞-fast, or ∞-thin $\Rightarrow$ all equivalent), can show

$$S_T = S_L \left(1 + \frac{u'}{S_L}\right),$$ no in the

limit for strong turbulence $u' \gg S_L$ ($u' \to \infty$):

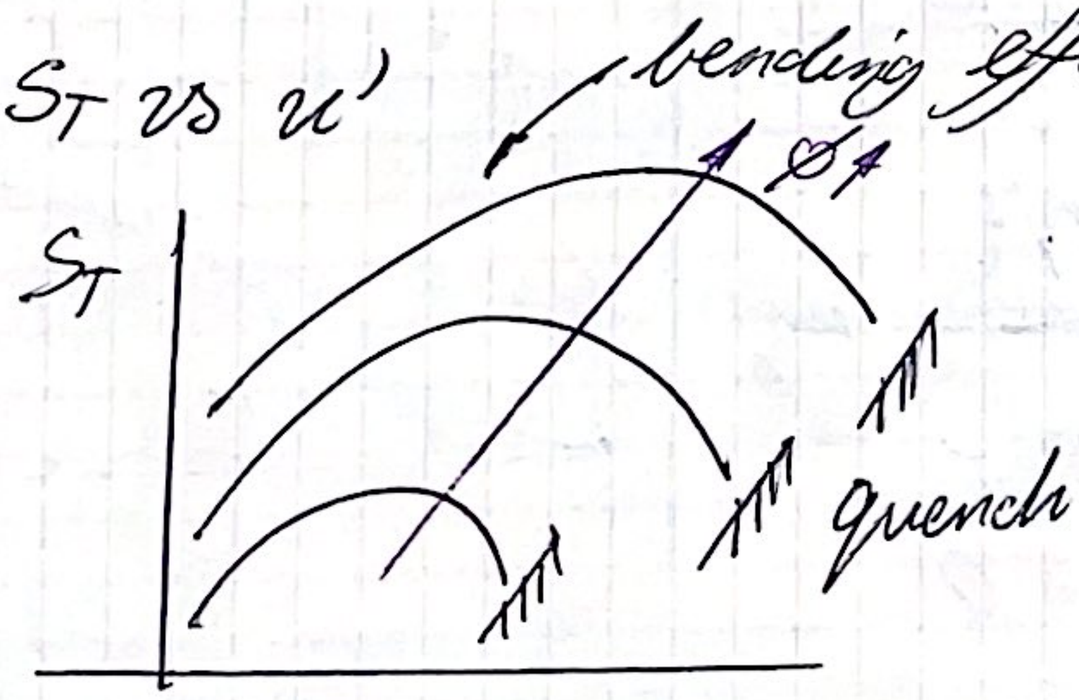
$S_T \approx u'$ which is saying that if turbulence is strong, the turbulent flame speed is close to oncoming eddy speed.

• ~~For "flame stretch" or when~~ ~~$Ka \gg 1$~~

• If $Ka \gg 1$ so when turbulence affects preheat zone:

$$\frac{S_T}{S_L} = \sqrt{D_T / \alpha}$$

11. S_T vs u'



Residence time is not affected by ~~stretch~~ turbulence (only by stretch) So just turbulence won't quench you.

But high turbulence means faster drift away of radicals — that's what quenches you.

NON - PREMIXED FLAMES

1. Mixture fraction

$$Z = \frac{m_1}{m_1 + m_2}$$

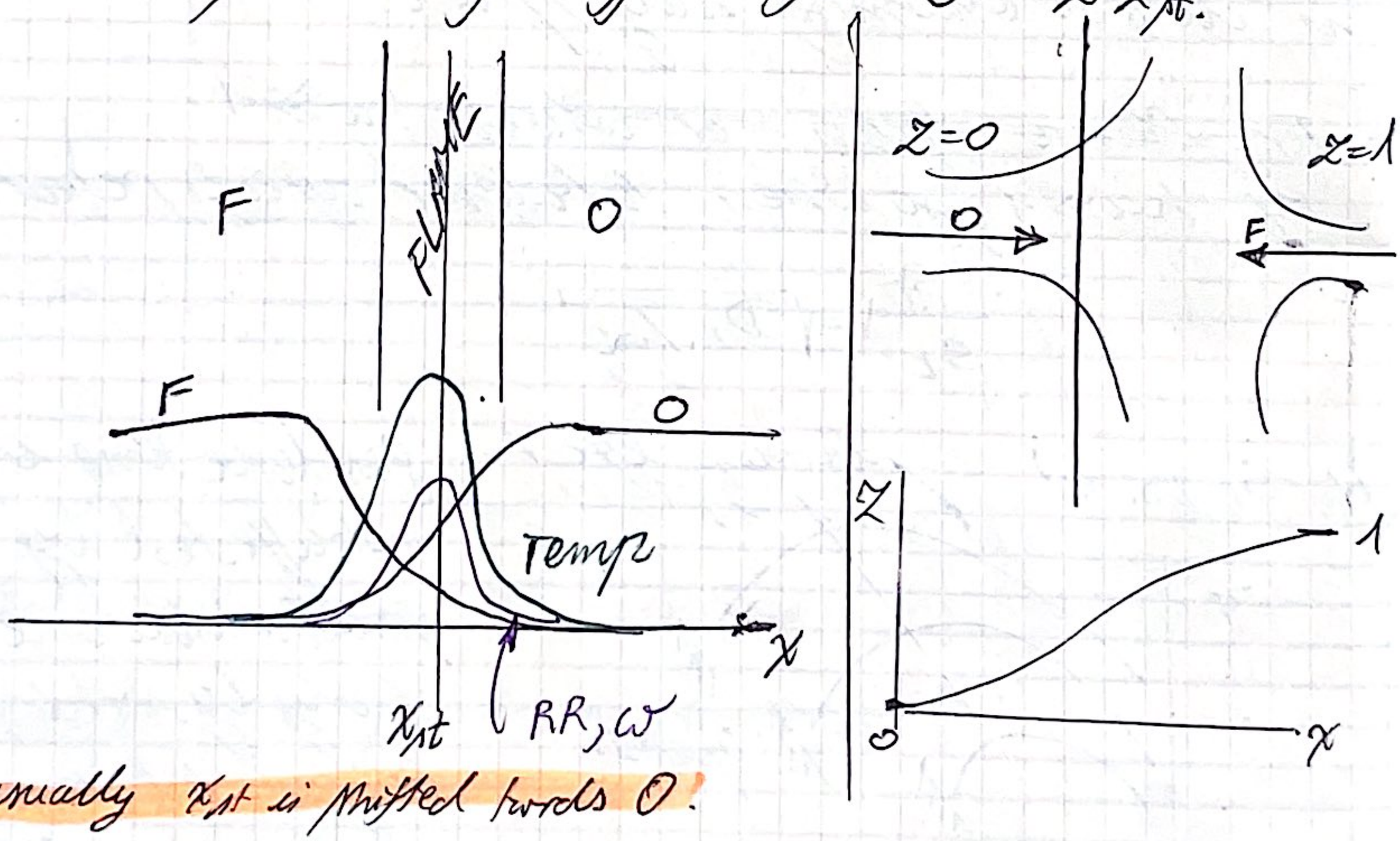
You want $Z = 0$ in air
$Z = 1$ in Fuel

~~m_{O_2}~~

and Z should vary continuously.

2. Diffusion flames do not benefit from a self-induced propagation mechanism — they're mixing controlled. The thickness of diffusion flame is not constant but depends on local flow properties

Internal structure of a diffusion flame



usually x_{st} is shifted towards O!

@ $Z = Z_{st}$ complete consumption of F & O is possible.

ei the definition $Z = \frac{m_1}{m_2 + m_1}$

$m_2 = s(Y_F^0 - Y_F) + Y_{O_2}$

$m_1 = s Y_F + (Y_{O_2}^0 - Y_{O_2})$, $s = \left(\frac{Y_{O_2}^0}{Y_F^0}\right)_{(st)} = \frac{\nu_{O_2}' W_{O_2}}{\nu_F' W_F}$

$\nu_F' F + \nu_{O_2}' O_2 \rightarrow P$

(more logically, Veynante:) or "

$$Z = \frac{\phi \frac{Y_F}{Y_F^0} - \frac{Y_O}{Y_O^0} + 1}{\phi + 1} \quad ; \quad \phi = \frac{Z}{1-Z} \frac{1-Z_{st}}{Z_{st}}$$

Y_F^0 is the fuel mass fraction in the fuel pipeline (usually 1 if only pure fuel flows there)

Y_O^0 is the oxygen (oxidizer) mass fraction in the oxidizer pipeline (e.g. in air $Y_O^0 \approx 0{,}23$). → not full air!

Verify that $Z(O) = Z(Y_F = 0; Y_O = Y_O^0) = \frac{-1+1}{\phi+1} = 0$

$Z(F) = Z(Y_F = Y_F^0; Y_O = 0) = \frac{\phi+1}{\phi+1} = 1.$

Notably the mixture fraction satisfies ~~the equivalent to global continuity (w/o source term!)~~:

$$\frac{\partial Z}{\partial t} + \nabla \cdot (\quad$$

in between "momentum" & continuity ("balance of Z"). notably — without a source!

(1) $\frac{\partial}{\partial t} \rho Z + \nabla \cdot (\rho v Z) = \nabla \cdot \rho D_k \nabla Z + \underset{\text{SOURCE!}}{NO}$

ASSUMING no diff. diffusion

i.e. when $D_k = D \; \forall k$.

Additional conservation eqns may be written down to give (Veynante)

(2) $Y_O(x,t) = Y_O^o \overbrace{(1 - Z(x,t))}^{\text{mixing}} + \overbrace{\frac{2_O}{2_F}\frac{W_O}{W_F}\left(\frac{q}{\phi}\right)\left[Z(x,t)(T^o - T_O^o) + (T_O^o - T(x,t))\right]}^{\text{combustion}}$

and a similar one for Y_F.

Using these relations, the combustion of diffusion flames may be broken down/ separated using the mixing fraction: combustion & mixing. Further, these 2 eqns the diffusion flame is fully resolved if Z and any of T, Y_F, Y_O is known.

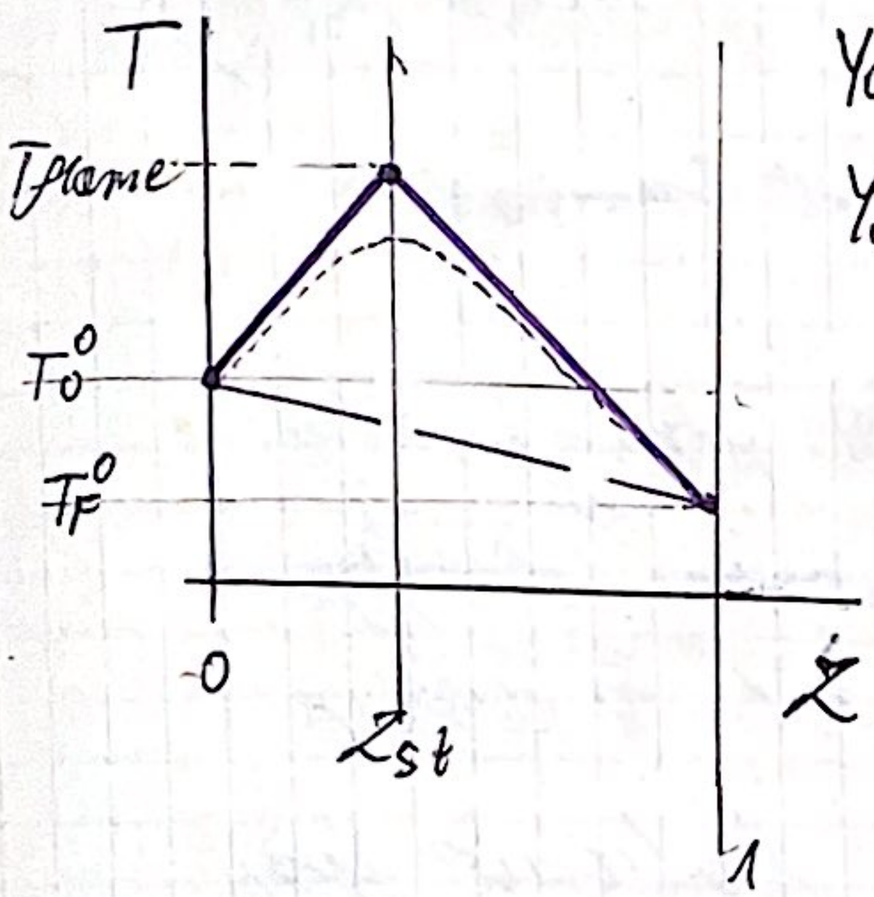
3. The classical definition of $Z = \dfrac{\phi \frac{Y_F}{Y_F^o} - \frac{Y_O}{Y_O^o} + 1}{\phi + 1}$

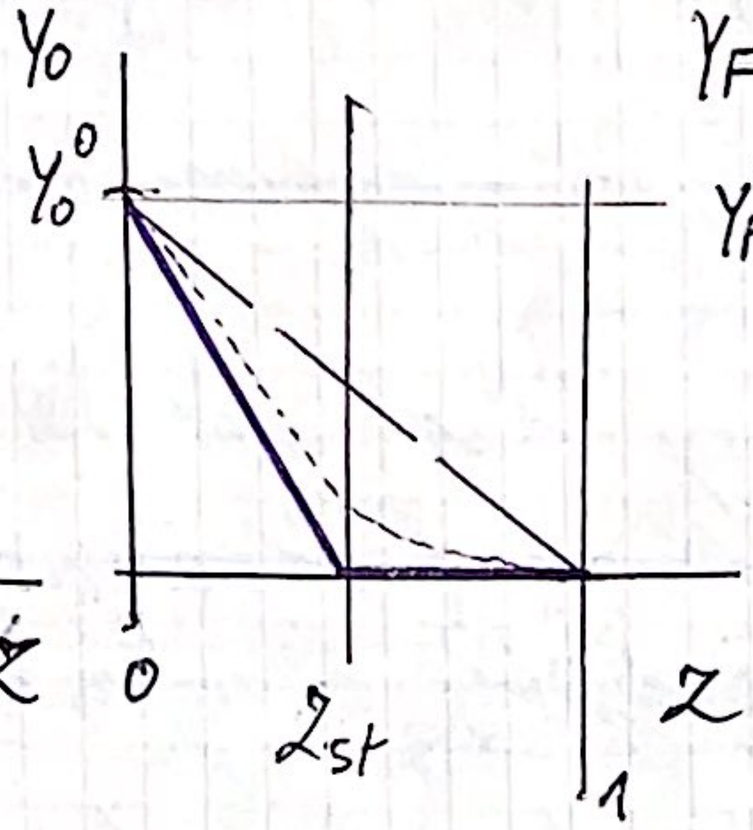
may be difficult to measure. Still, we need to come up with a variable under of Reaction itself → Dilges mixture fraction

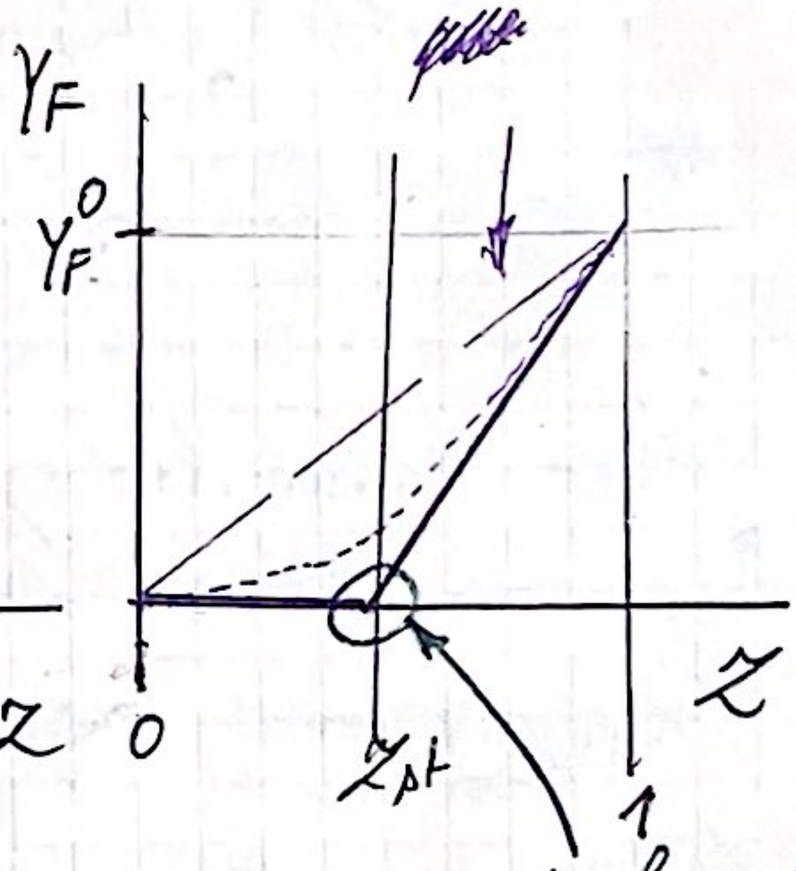
$$Z = \frac{\beta - \beta_2}{\beta_1 - \beta_2} \quad \text{again is to vary } 0,1 \qquad O \to F$$

It's the same as it was before except now it takes into account $W_K, 2_K$ (scaled versions)

4. Burke-Schumann flame Structure







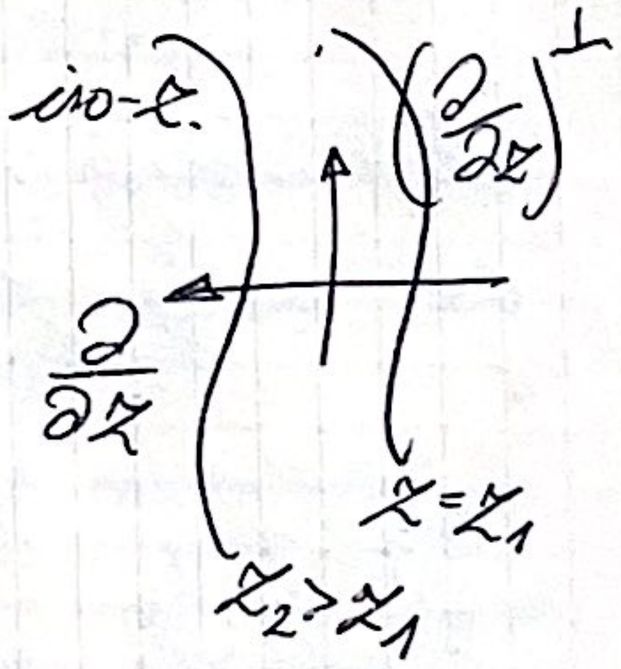
——— ——— ——— = pure mixing, no CC

- - - - - - - - - - - - = equilibrium, ∞-fast (diss.)

——— = one-step chemistry, ∞-fast (no diss.)

fuel gets completely used @ z_{st}
left, no fuel, right, interpolate with Y_F^0

5. The mass balance (1) & temp eqns (2) may be rewritten in a coordinate system spanned by $\frac{\partial}{\partial z}$ & $\left(\frac{\partial}{\partial z}\right)^\perp$



The balance then becomes (vgrunte)

$$s\frac{\partial Y_i}{\partial t} + s u_\perp \cdot \nabla_\perp Y_i = s\chi \frac{\partial^2 Y_i}{\partial z^2}$$

$$+ \nabla_\perp (sD\nabla_\perp Y_i) - sD\nabla_\perp(\ln|\nabla z|)\cdot\nabla_\perp Y_i$$

$$+ \omega_i$$

where $u_\perp$ are the velocities in direction $\left(\frac{\partial}{\partial z}\right)^\perp$ & $\nabla_\perp$ is the gradient along $\left(\frac{\partial}{\partial z}\right)^\perp$.

$\chi := 2D|\nabla z|^2$ is the scalar dissipation rate

SDR measures the inverse of diffusive time $\tau_x = x^{-1}$. As $\tau_{x\ell}$, mass & heat transfer through the cio χ-surfaces are encased

When curvature of χ is not too strong, the $\nabla_\perp \ll$ other terms (fluctuations along $(\partial/\partial z)^\perp$ are negligible compared to other terms), so the transformed balance eqn reduces to:

$$\boxed{S\frac{\partial Y_i}{\partial t} = S\chi\,\partial_z^2 Y_i + \dot{\omega}_i}$$

If unsteadiness is neglected, the mass & temperature balances become:

constant Le assumptn!

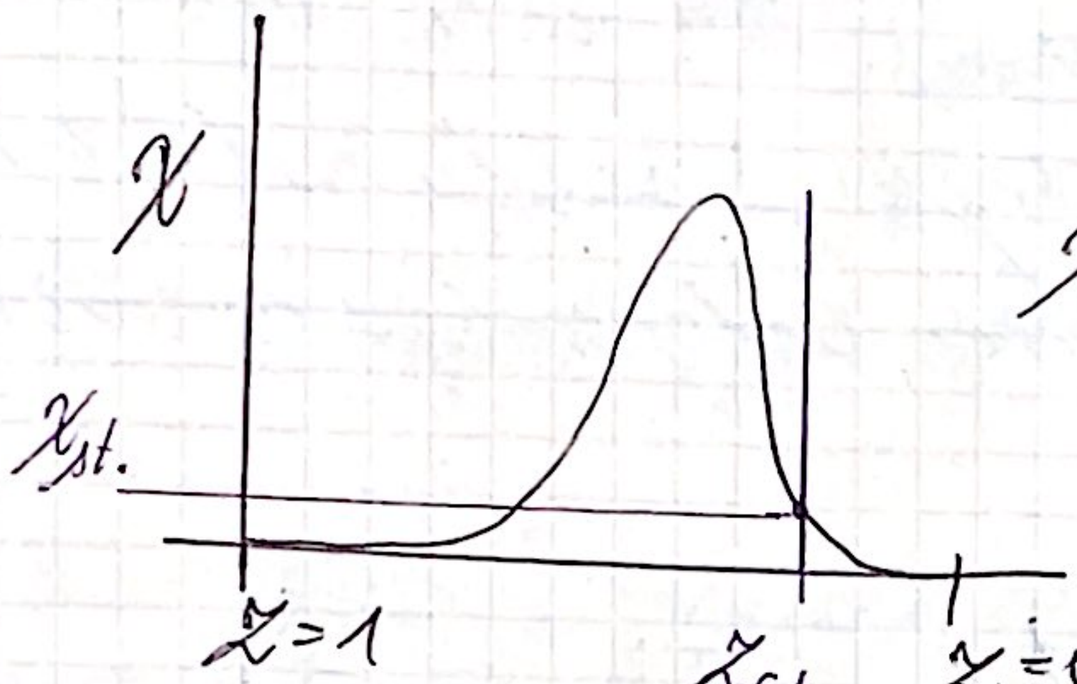
$$\boxed{S\chi\,\partial_z^2 Y_i + \dot{\omega}_i = 0} \quad \text{("continuity")}$$

$$\boxed{S\chi\,\partial_z^2 T + \dot{\omega}_T = 0} \quad \text{("energy eqn")}$$

Meaning that concentrations & temperature are only fns of z & χ: $Y_i = Y_i(z,\chi)$. $T = T(z,\chi)$

Knowing $\chi = \chi(z,t)$ is difficult but $\exists$ methods to approximate it. Most important is $\chi_{st.} = \chi(z_{st}, t)$, which measures heat & mass flux through the stoich. surface.

One method to know $\chi = \chi(z, t)$ is from asymptotic studies. Result: (Peymante):



$$\chi = \frac{a}{\pi} \exp\left\{-2\left[erf^{-1}(1-2z)\right]^2\right\}$$

Closing comments:

- there are 2 limiting (boundary) cases:
  1) $\chi \ll$: mass & enthalpy fluxes are so fast the rn may be considered as equilibrium (----- line from Burke-Shuman)
  2) $\chi \gg$: extinction is observed & pure mixing with no reaction is observed

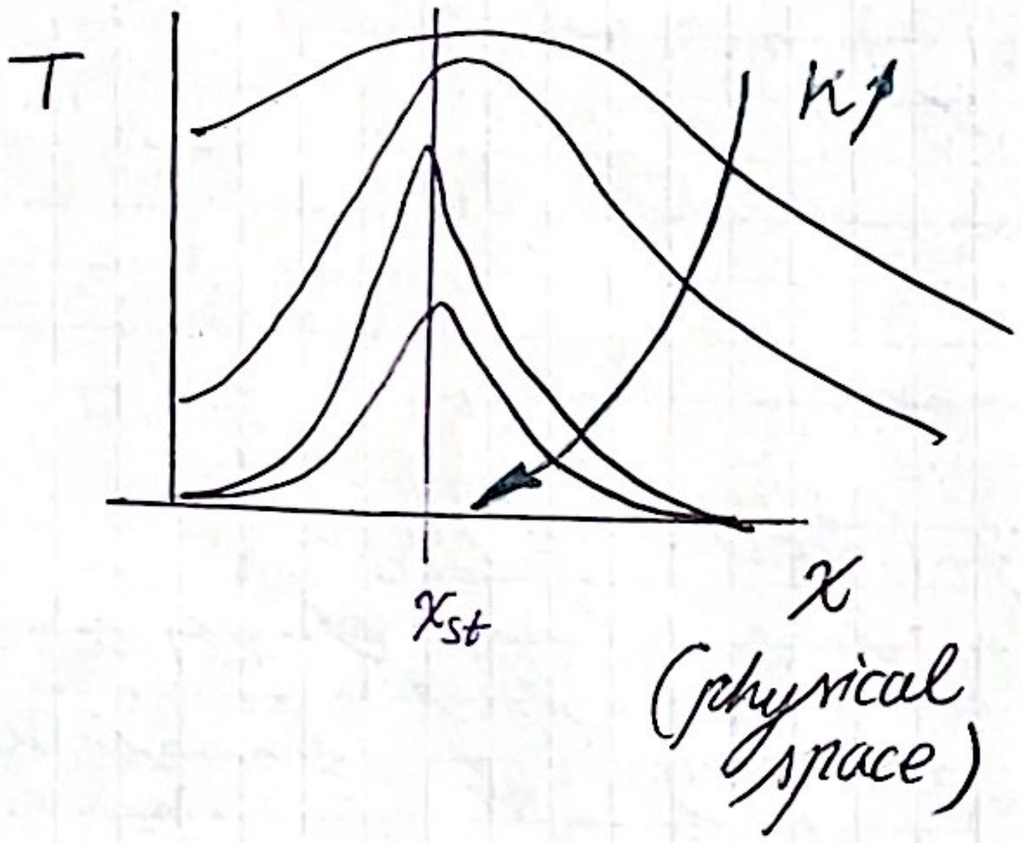
Note how the above makes sense:

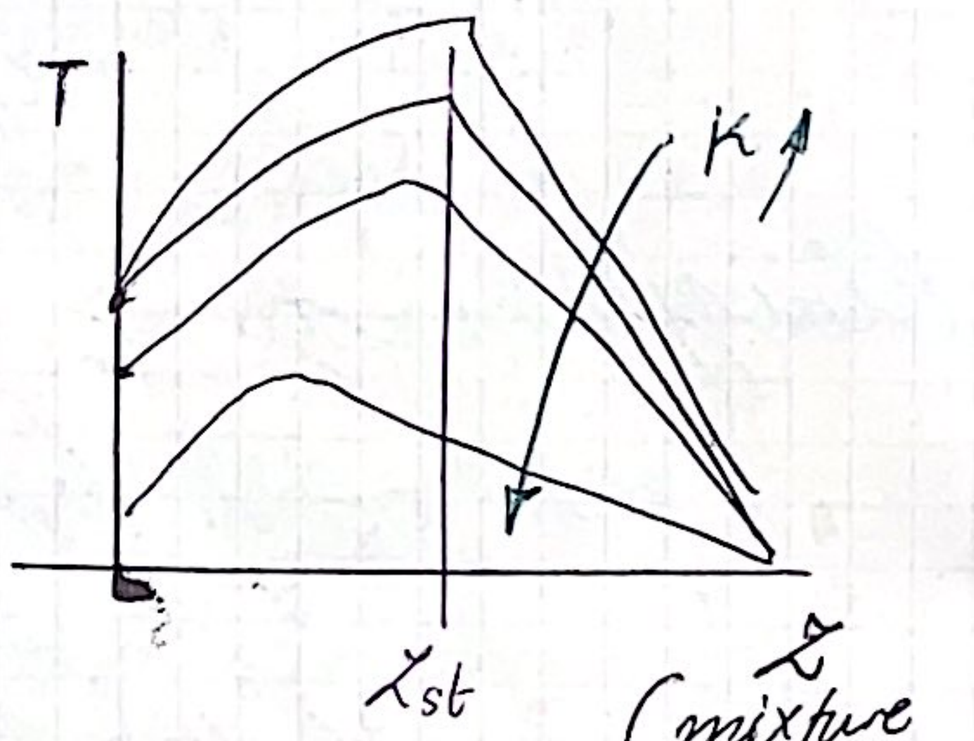
If 1) $\chi \ll \Rightarrow \tau_{mix}$ is huge compared to τ_{chem}, or chemical time is so-fast $\Rightarrow$ by def equilibrium. Conversly, if

2) $\chi \gg$, then τ_{mix} is super fast ($\tau_{mix} \ll$) compared to τ_{chem} so before any reaction takes place, it's immediately mixed $\Rightarrow$ perfectly stirred reactor: $Da < 1$ $\Rightarrow$ extinction.

- The above doesn't take into account 2D effects ($\nabla_\perp \equiv 0$ assumption) or sinks (radiation). In such cases these solutions / eqns shouldn't be used & we need further independent variables.

6. Results.



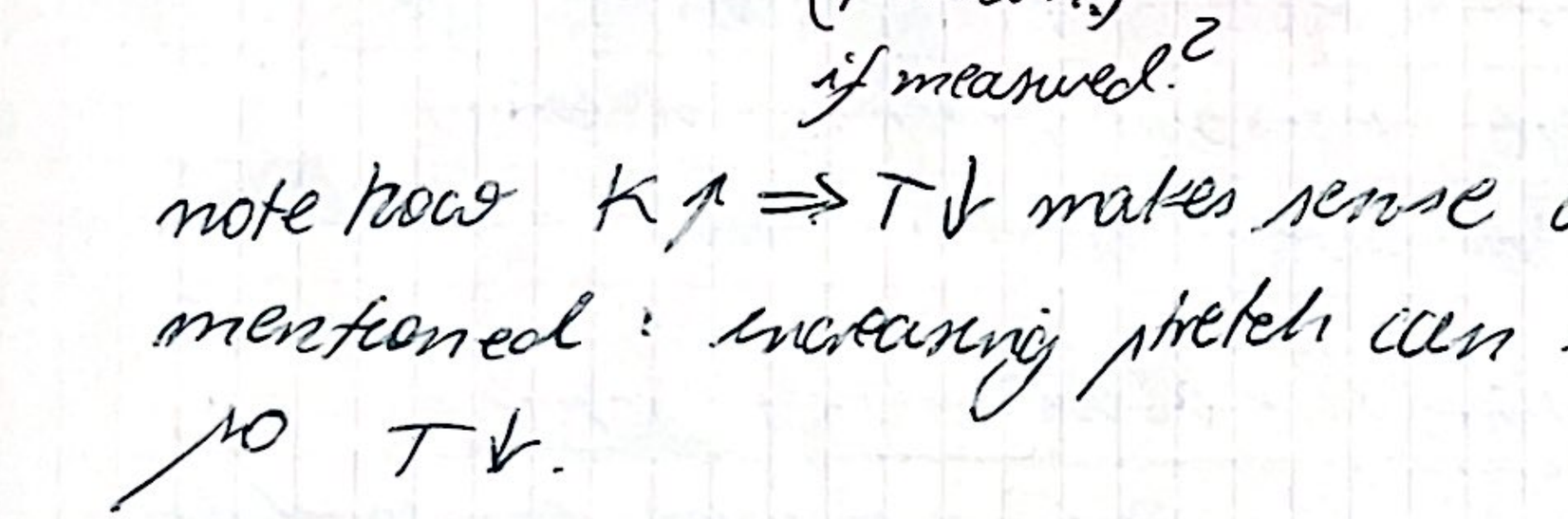


$T(x) \longrightarrow T(z)$

$z = z(x)$ (known?) if measured.[2]

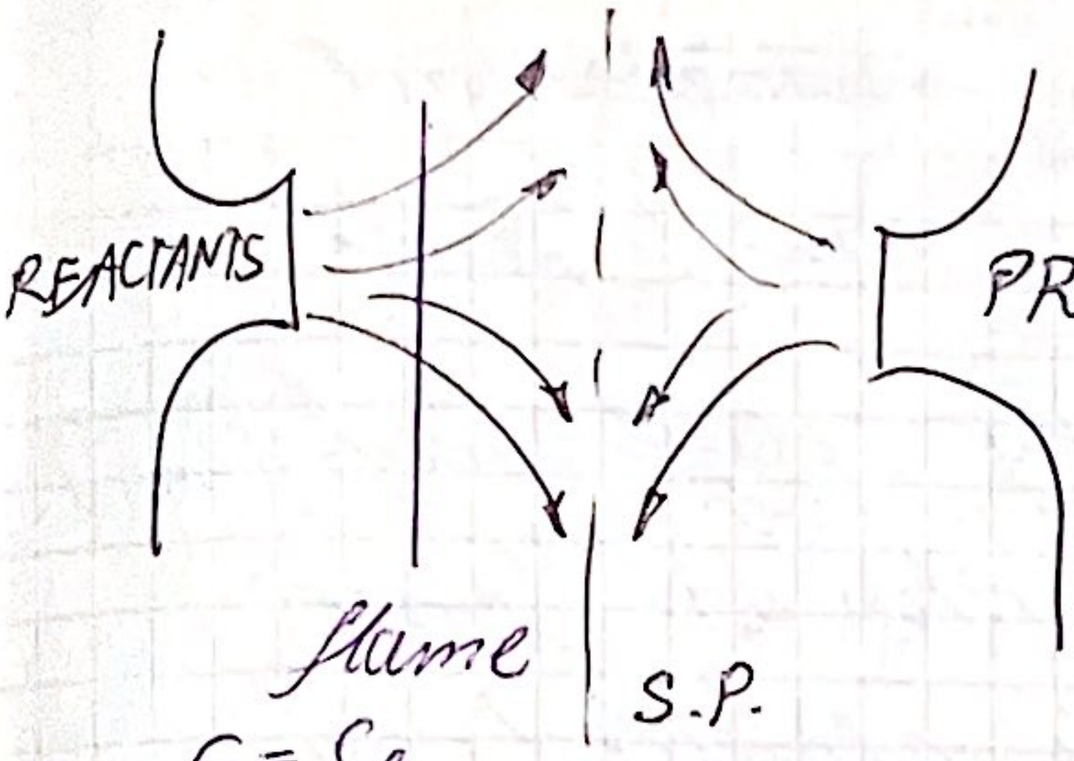
note how $K\uparrow \Rightarrow T\downarrow$ makes sense as it has been mentioned: increasing strain can lead to quench $\Rightarrow T\downarrow$.

2. Opposing jets / counter flow:



why shifted?[2] look @ $\left(\frac{Y_F}{Y_O}\right)_{st}$ and how s_O, s_F change along y/z

DIFFUSION FLAME



PREMIXED

i.e. "recirculation of products"

note that shooting products @ reactants stabilizes the flame in the sense that it keeps it alive — it provides hot gases so enthalpy which prevents quench (you provide energy energy to "keep-it alive"). That's why introducing swirl en CC's is beneficial ("stabilization by swirling jets" → see lecture (11)).

Veynante: "Many flames in burners are stabilized by the recirculation of burnt gases, leading to stabilization mechanisms controlled by the mixing between fuel, oxidizer & burnt gases".

8. Effect of stretch in diffusion flames

- Diffusion flame is not able to change its position unlike freely propagating laminar flame — it's "restricted" in a way. As a consequence, in case any strain is applied to it, the flame can't run away from it and is forced to thenitself —

meaning $t_R \downarrow$, heat losses, ~~reactants~~ and so extinction can happen much faster compared to premix. Lastly, differential (or preferential) diffusion is not linked to stretch as it is the case for premix, although it's effects can be relevant.

Lecture 14 — Turbulence Modeling & Chemistry Interaction

6. In LES $\bar{S}$ changes only if $M > 1$, but in CC $\bar{S}$ varies cuz of temp change & that causes some unclosed terms

To close it, apply a mean filter: $\bar{\dot{\omega}}_k = \overline{\frac{S\dot{\omega}_k}{\bar{S}}}$ normal filter / Re filter.

Then you avoid additional unclosed terms but the downside is your properties are all density weighted

Problem is Arrhenius modified eqn cuz approximately

$$\bar{\dot{\omega}} \neq A \tilde{T}^{\beta} e^{\frac{-E_a}{R\tilde{T}}} \overline{[X_A][X_B]}$$

So must either use DNS or other modeling approaches (I think the one on the slide didn't work)

I think this would suppress the peak concentrations

7. Remember - FDF (subgrid PDF), filter density fn

8. $\frac{\epsilon}{k}$ = "k-ϵ"

9. Defn of filter $\bar{\omega}_k = \int \omega_k(\psi) \underbrace{\tilde{P}(\psi; x, t)}_{\text{PDF, not known}} d\psi$

Don't mind the huge expression, you can't solve it cuz of some diffusion (∇) → you need to simplify

10. Simplifications → Pope uses Monte carlo. Inject particles & track w Lagrangian form. Problem is you don't know μ, can model, but it's super expensive to approximate the PDF. Sometimes even more expensive than DNS. But if you do it successfully then can recover PDF

"engage" 2.

13. Solve upto 8 eqns ~~(fields)~~ with different stochasticities (randomness). They'reall flamelets, but ~~the avg~~ if you take the avg of these 8 solns (fields), then you reconstruct $\tilde{T}_k = \int \dots dZ$! (can be proven)

Disadvantage → you need @least 4-8 eqns using Arrhenius form

15. Just remember the main idea behind the method → use flame thickening so you don't face the fundamental problem of "fluctuations" (?), you can still use Arrhenius.

20. Just like in the Peters diagram - the small vortices either are not strong enough or small enough to get into the flame and change it's internal structure. If you take a cut it's looks the same everywhere.

So the external structure is laminar - I can solve it precompute it using a 1D soln. (lookup table)

21. @real won't expect to write down the eqn, just gotta know what it is — transport eqn for the progress variable (c). For non-premixed you also have a transport eqn but for mixture fraction (Z)

Once solved, can reconstruct the external structure of the flame using c (or Z).

22. Incase of non premixed one variable c is not enough - you need Z & ~~scalar dissipation rate~~ (20)(21)(22)

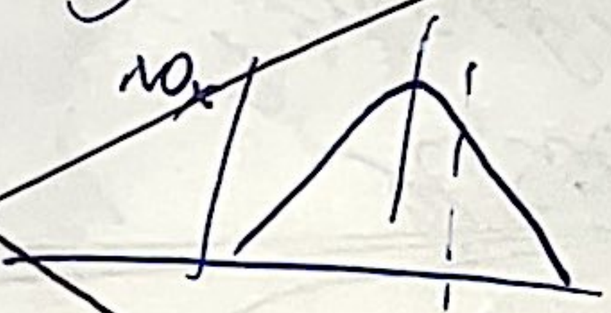
(or strain ~ SDR)

$N_e = D_e \nabla c \cdot \nabla c$.

Check if strain is tangential

Comb Q&A

① NOx peak LEFT of $\phi = 1$



why? cuz need high Temp but also more oxygen so $\phi < 1$.

② With hydrogen you don't (need) to quench cuz mixing is super fast so $t_r \ll$. ($Le_{H_2} \leq 0.3$)

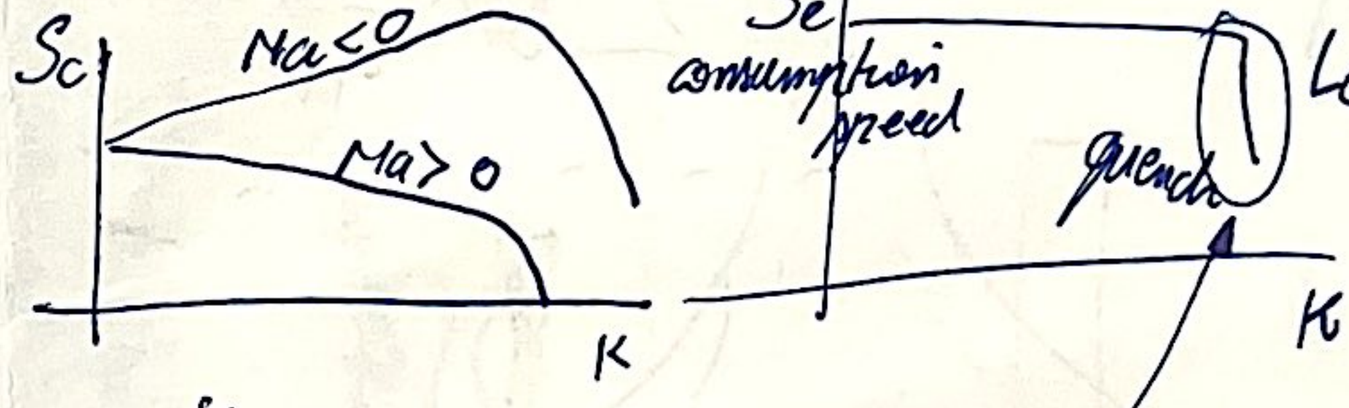
③ R ⟶ ⟵ P (Swirl burner)

also in CC,

P shoots reactants stretches the flame which means longer flame which means lower temp. so lower NO_x! Stabilizes flame cuz you provide enthalpy (keeps flame alive).

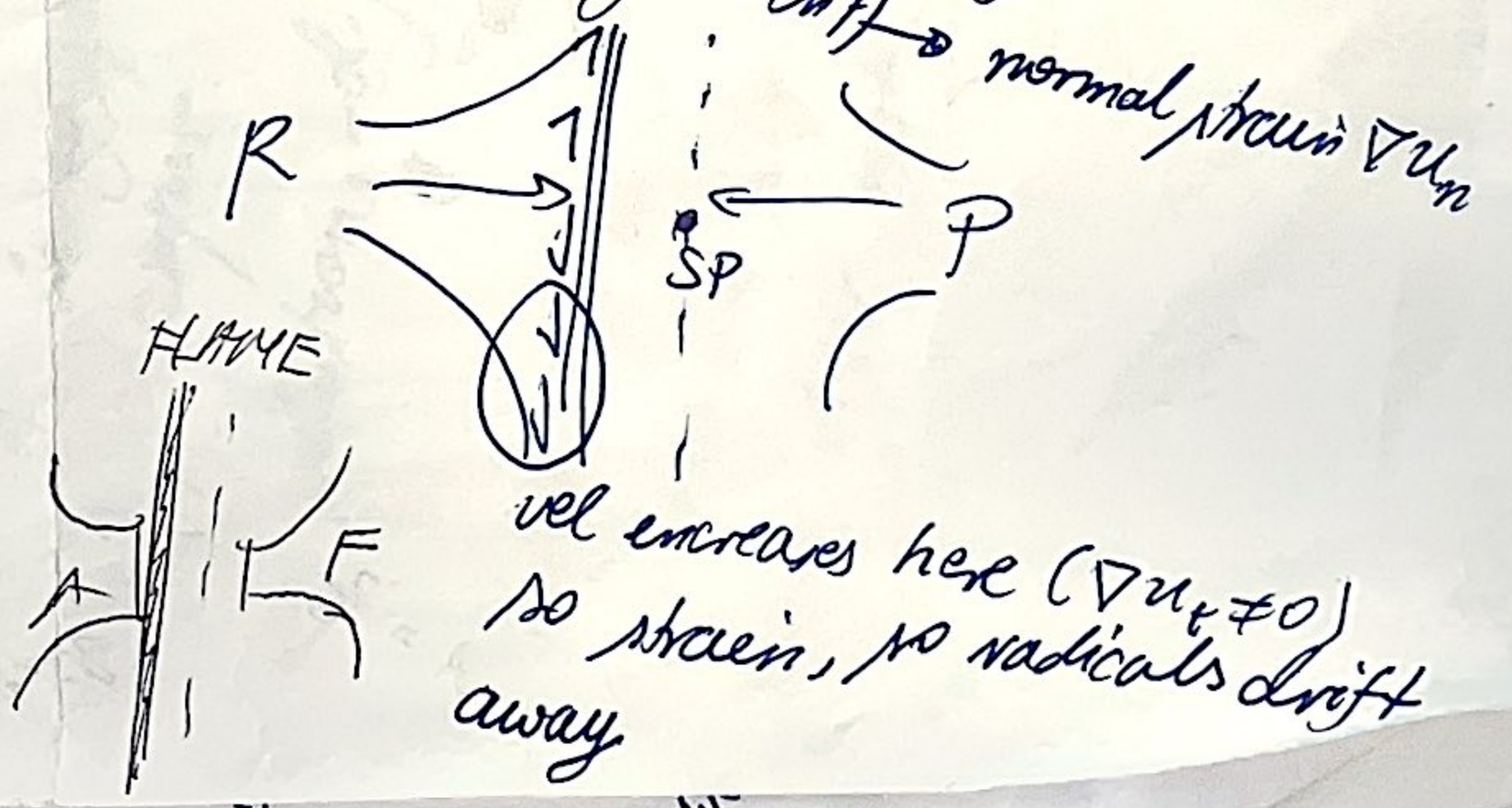
Effect of strain tangential is to increase flame surface.

If normal strain — change residence time. If flame non premixed, it happens immediately, if premixed, it takes a while.



if ∞-thin flame then $t_r = 0$ (∞-fast, ∞-gradient)

accelerate thru flame too quickly ineff combustion



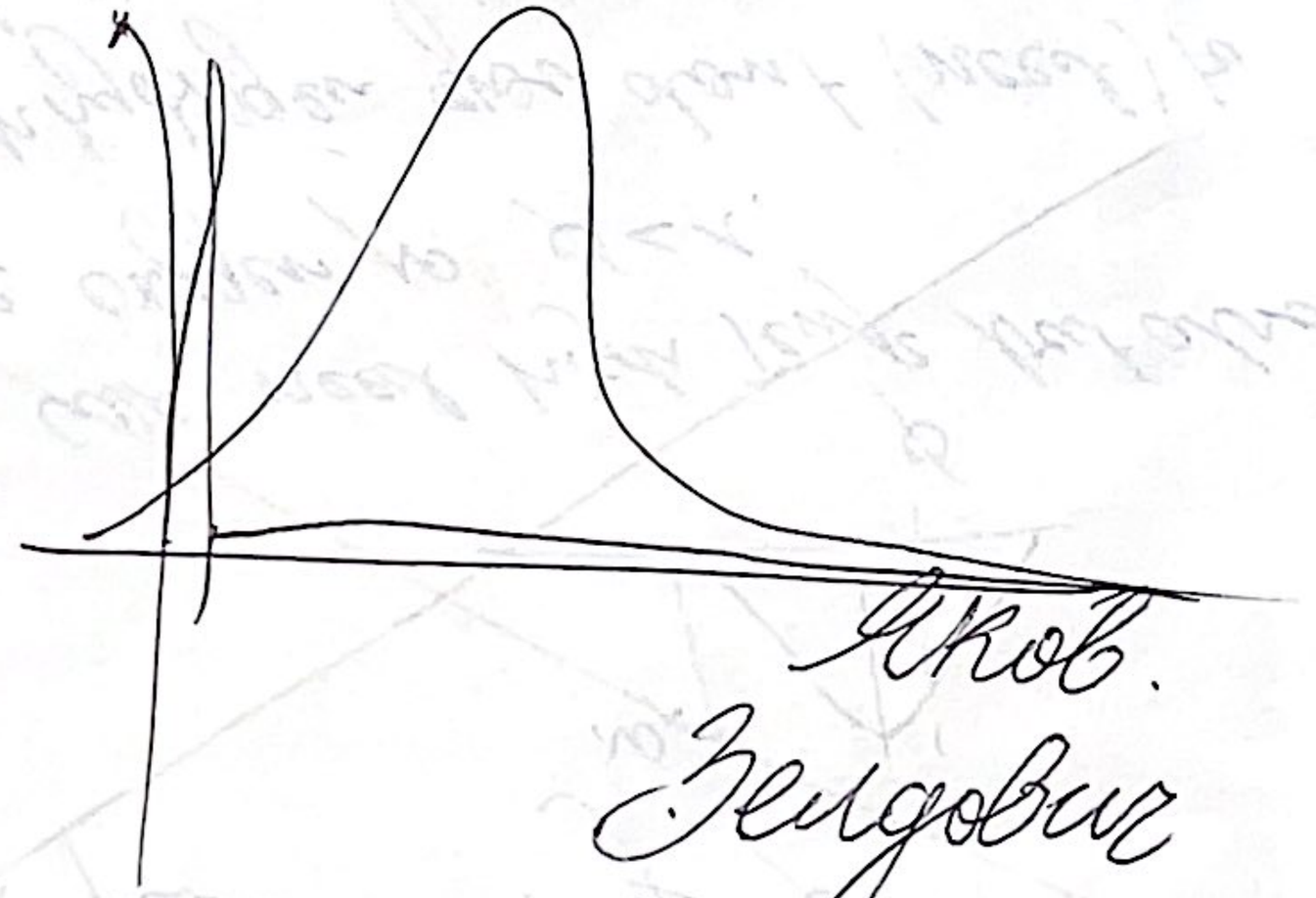
vel increases here ($\nabla u_t \neq 0$) so strain, so radicals drift away

Т Е З Яков Зелдович.

Зелдовича Зелдовича.

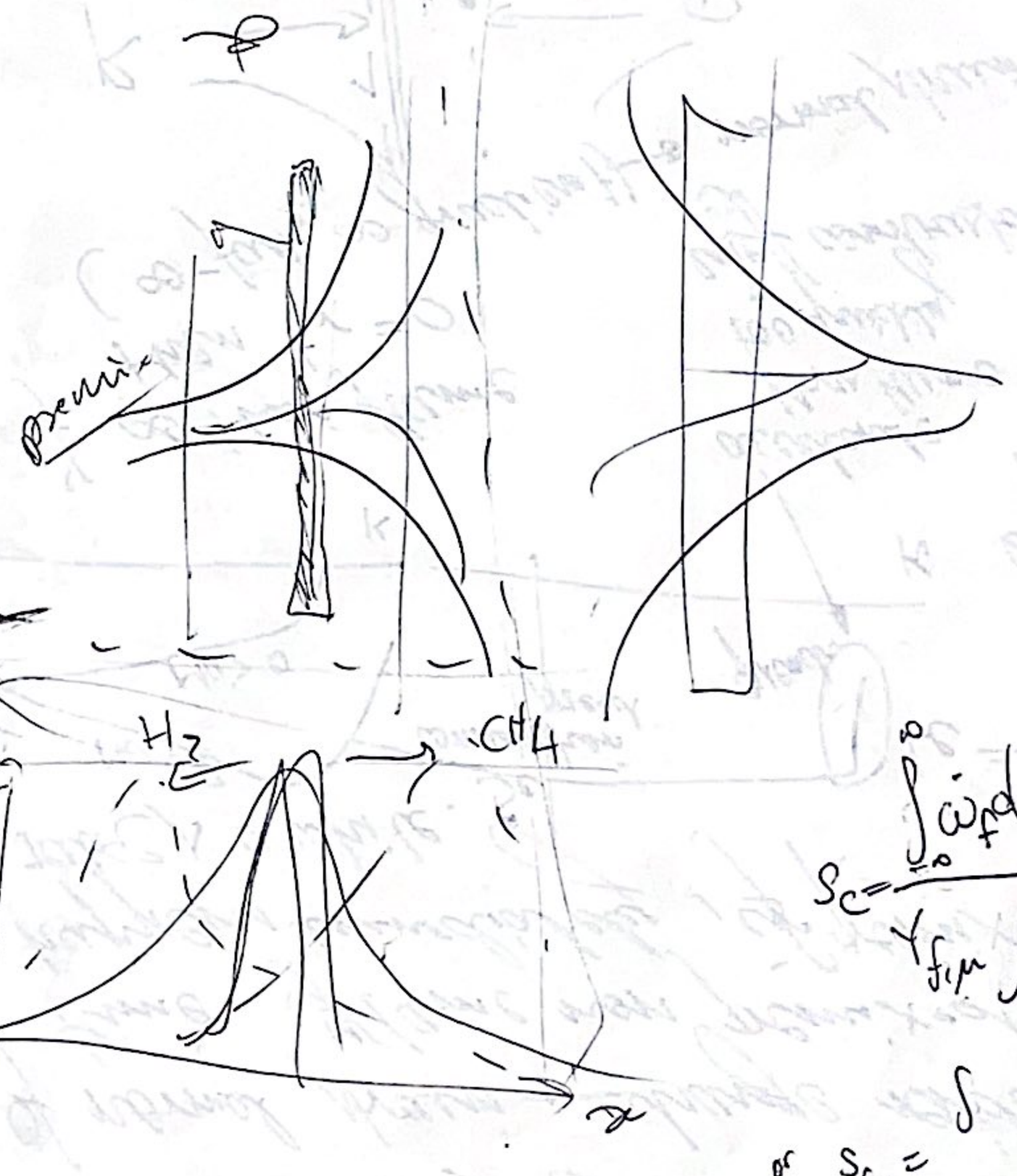
У Г М Г Ц

$P = \dot{m} \cdot L_{HV}$



Яков.
Зелдович

Зелдович



$$s_c = \frac{\int_0^\infty \dot{\omega}_f dn}{Y_{f,\mu} \rho_\mu}$$

or $s_c = \int$

Purdue

24. You assume a shape of the PDF. This shape needs to be second order which means need to depend on

$E[c] = \tilde{c}$ & $Var(c) = \tilde{c''^2}$ Unless non premixed

You need $2 \times 2 - 1 = 3$, or $Var(\tilde{c})$ not needed! ← or SDR.² (one of them)

So then you have the fn (lookup table) dependent on E & Var: $\tilde{\dot{\omega}}(\tilde{c}, \tilde{c''^2}) = \int_0^1 \dot{\omega}(c) P(c; \tilde{c}, \tilde{c''^2}) dc$.

2 or 3 variables.

" "

$\tilde{c}$ you know cuz it appears in eqn of Sicle $\tilde{c}$.

it's the unknown you gotta solve for. Var(c) you don't know, you can set a transport eqn for it or somehow else.

28. Your table becomes 4 or 5 dimensional, so ← if you use covariance (necessary for RANS LES — NOT) it takes lot of space & gotta interpolate so might defeat the purpose.

30. One solution — different stretch!

1. diff diff effect
2. If mesh size to big

for future dev not important

THE END

31. Pu

Pyfanica

1. Skgd $\frac{\Delta n_k}{\Delta v_k} = const$ and how that implies

$$\frac{\Delta Y_k}{\Delta v_k} = const^2$$

2. Skgd $\sum_k \omega_k = 0$, for $\omega_k := \sum_j \omega_{kj}$

for $\omega_{kj} := \frac{dY_{kj}}{dt}$.

3. Derivery Gibbs you say assume $p = const$ but then the rates always fixed?!

4. LN p 35 2ND TE?

5. ~~Q7, Q8?~~

6. WHY? a When have lean or when NO is produced then can't use chemeq". Is it ab residence time? Too slow?

7. L3 s. 13 "Note $K_{pr} = K_c \times (RT)^{\Delta v}$" Skgd?

8. Why dquench behaves like L "6" - S33/48 (esp S2 of fuels) I thought it was other way 'round.

9. Why DIFF no FB while PREM prone FB? (+ stability?) + CO_2?

10. Q "12"

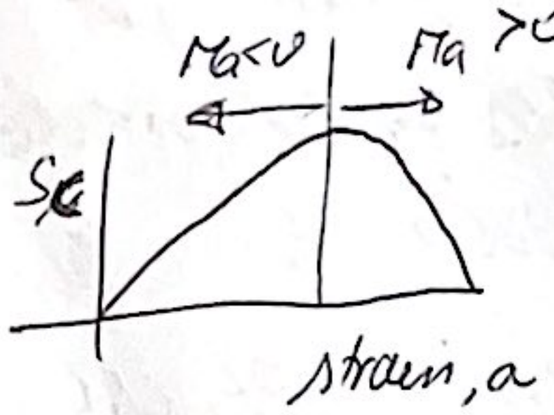
11. ~~em prem also BB radiation~~ diff also radicals so why don't see peaks? Cuz they smaller than BB peak?

To remember

1) $Pe = \frac{\chi_f}{\delta_L}$

2) $\omega_{DL} \propto S_L \cdot K$
$\propto \sigma = s_u / s_L$

3) "flame transfer fn"

4) 

5) AXIAL INJ
H_2O INJ
STRAIN LOCK
MIX. F.
TRAPPED V-TEX W T-CTRL
↳ P&C

6) Favre: ~~Favre decomposition~~
$\tilde{Q}'' \equiv 0$; $\tilde{Q} := \frac{\overline{\rho Q}}{\bar{\rho}} \Rightarrow$ ~~$\overline{Q''s''} = \overline{Q''}\,\bar{s} = 0$~~

7) unclosed $\overline{\dot{\omega}_k}$ in local mass, not en.

8) "flamelet" only exists in PREM!!!

9) EBU: $\overline{\dot{\omega}} \approx - C_{EBU} \frac{\varepsilon}{k} \bar{s} \bar{Y}_k (1 - \bar{Y}_k)$ → fast so com: can't capture sloo

10) FDF: $P(\psi, x, t)$ is JOINT PDF ; $\psi = \omega + Brown.$

11) AFT: F to enflate D_t & $\frac{1}{F}\omega \oplus E_T$ in D_t & $\frac{E_T}{F}\omega$ ← counteract eroding small wrinkles, efficiency boost
ONLY PREM.

12) FSD: $\dot{\omega} = \Sigma \cdot s_L \cdot S$; $s_T = s_L \frac{\Delta}{s_u}$

13) $S_{DNS} < S_{LES} < S_{RANS}$

14) convergence: $\forall grid, \Delta_{grid} \to 0$
consistency: $\Delta_{LES} \to 0$

} turbulent flame speed closure — use exp & /and empirical relations: $s_T = s_T(s_L)$ (algebraic). Based on understanding that turb. wrinkles & stretches the flamefront & that $s_T = fn(s_L)$.

15) Flamelet model: $Q = Q(c)$ ← PREM ; $Q = Q(Z, \chi)$ ← NONPREM (or strain outlook is also ok.)

16) FGM is FM
technique. theory
numerical.

17. ! flamelet paradigm ! (dem. ~ fast, no affect of wrd structure)

MODELS (2)

① Laminar flamelet model → solve a family of SS, 1D flames parametrized by χ(diff) or c(prem.). Transport $(c, \bar{c}, c')$ or $(z, \bar{z}, z')$.

② FGM → similar to ① but uses more than 1 dvt variable @ a time $(z, c, \bar{z}, \bar{c}, c', z')$ of a time. Used for ~~premixed~~, partially premixed, or if $\tau_{chem} \neq 0$.

CLOSURES: Presumed PDF closure — can be applied to laminar flamelet model ⊙. (not a model itself) just a "help" for other models. You have to use it to solve transport of all variables — the source term:
- if closes $\dot{\omega}$ ⊙. Note $\dot{\omega} = \omega(c, z, \dots)$
- but you need $\tilde{\dot{\omega}}$ not $\dot{\omega}$. So assume $\exists P$ s.t.

$$\tilde{\dot{\omega}} = \int \dot{\omega} P(\text{⊙}\, dc\, dz + d\tilde{z} + d\tilde{c}'')\, dc\, dz^* \quad , dc \in (c, z)$$

Without it, you must solve full transported PDF which is unrealistic. So it's an alternative for transported PDF-OR EBU.

8. Hydrogen modelling
- ⊙ $\Delta_{grid} < \delta_L \Rightarrow$ correctly predicted ⊙ as long as s correct. TPinstab
  only ⊙ problem if high curvatures (use 2D then)
- $\Delta_{grid} > \delta_L \Rightarrow$ must model ⊙ TD as $\omega_{tot} = f(K)$, $\forall K < grid$
- ⊙ in case autoignition: $\omega_{tot} = A \cdot \omega_{prop} + B\, \omega_{autoign} + \nabla \cdot \delta x$

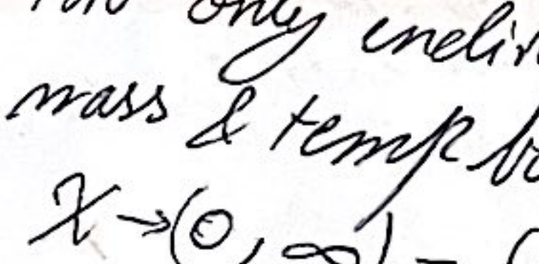
19. s_d measures deviation of fluid vs flamelet (projected onto n)
20. $Ka = K \cdot \frac{\delta_L}{s_L^0}$
22. "Flame speed closure" → hydrodyn: $s_T = s_L \left(1 + \frac{u'}{s_L}\right)$
23. Turb only indirectly quenches you: by stunning (if not ∞ thin) AND faster drift away of h & *.
24. mass & temp balance in $(\partial_z, \partial_z^\perp)$: $s \partial_z Y_i = s \chi \partial_z^2 Y_i + \omega_i$
25. $\chi \to (0, \infty) =$ (equilibrium & extinction)
26. nu panico:

$$CH_4 + 2(O_2 + 3{,}76 N_2) \to 2H_2O + CO_2 + 7{,}42 N_2$$

lean: $\phi CH_4 + 2(O_2 + 3{,}76 N_2) \to 2H_2O + CO_2 + \left(\frac{2}{\phi} - 2\right)(O_2) + \frac{2}{\phi} \cdot 3{,}76 N_2$

rich: $\phi CH_4 + 2(O_2 + 3{,}76 N_2) \to (\phi - 1) CH_4 + 2H_2O + CO_2 + 7{,}42 N_2$

27. g) → stability (cellular) @ $\phi < 1$ lean $Le_{H_2} \ll 1 \Rightarrow$ unstable (RQL good, lean bad)
→ Stab(FB): @lean prone to FB, @rich no.

28. 

29. Cp CO_2 37
Cp CO = 29

30. $\delta q = dh = du + v dp + p dv$
"why ⊙ @ rich don't add work?"

31. RO ≠ DOR

32. diff always more not

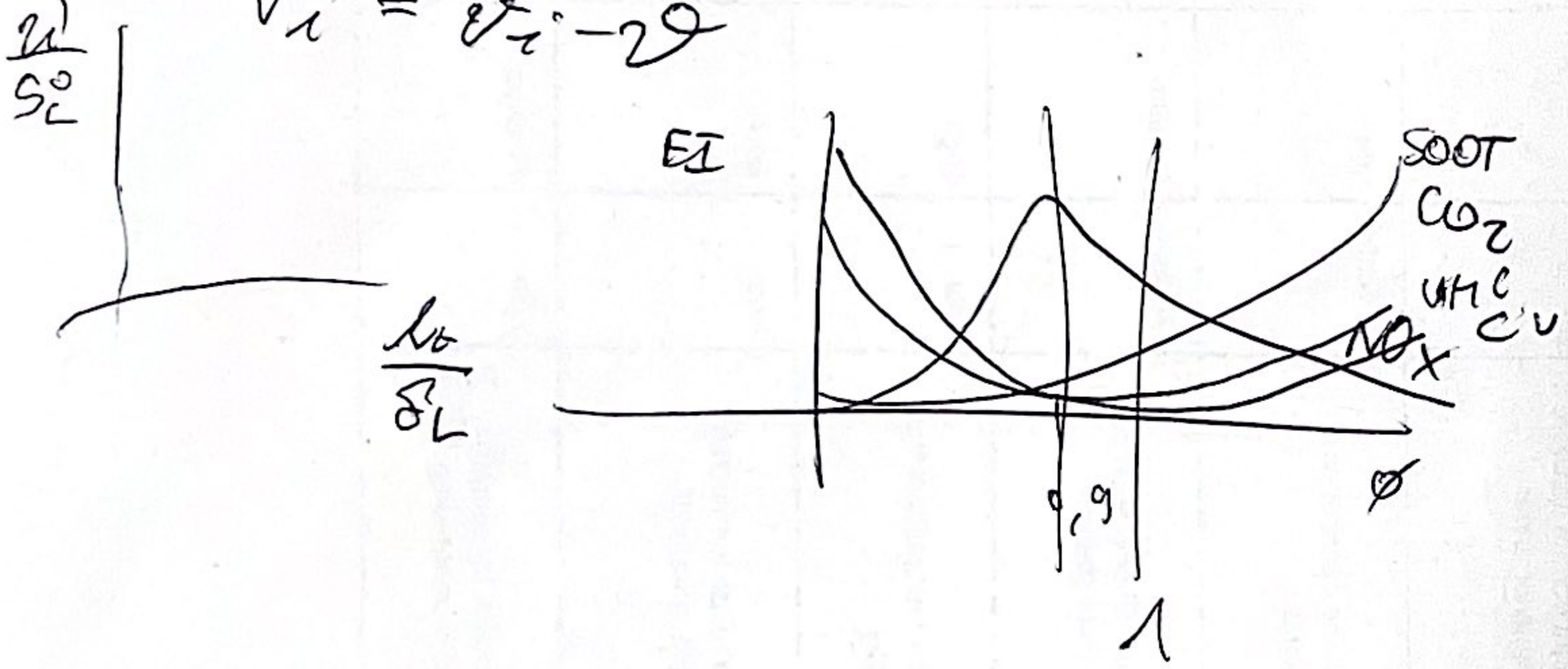
$$j_{in} = -\rho D_i \nabla Y_i$$

$$j_{inv} = -\rho \nu \frac{d Y_i}{dy}$$

$$D_i'' = \frac{1 - Y_i}{\sum \frac{X_i}{D_i}}$$

$$v = \sum Y_i v_i$$

$$V_i = v_i - v$$



	z_{1i}	$\Delta x_i' C_2$	$\Delta x^2 n_i'' C_3$	$\Delta x^3 n_i''' C_4$
cu_1	α	0	0	0
cu_2	b	b	$\frac{1}{2!} b^2$	$\frac{1}{3!} b^3$
cu_3	c	$2c$	$\frac{2}{2!} c^2$	$\frac{2*}{3!} c^3$
	0	1	0	0

Q0 (L1, S33): What's the advantage of an isobaric process as cmp to isochoric one?

Q1(L2, S4): Why peak of $T_{ad}(\phi)$ not @ $\phi = 1$?

Q2(L2, S4): Would T_{ad} in an isochoric process be higher or lower

Q3(L2, S4): Is higher T_{ad} better to get energy? (Assume: mech. en. in an ideal cycle)

Q4(L2, S5): Why T_{ad} ↑ if p↑?

Q5(L2, S8): Are these temps accurate (T_{ad} from heat balance). What are we missing?

Q[a] (LN, P.32). Determine if free energy is larger for an isobaric or isochoric proces?

Q6(L2, S13). What does $\Delta G = 0$ mean?

Q7(L2, S18). How does T_{ad} ↑ with reactants temp?

Q8(L2, S18) Are species well predicted w/ the equil. assumption?

Q9(L3, S22) Why η_g ↓ with X_{O_2}, p & T? (up to some pt)

Q10(L4, S12) Why we want high pressure @ entrance to cc. Why do isobaric cycles diverge?

Q11(L"6", S45) Do H_2 flames produce soot?

Q"12"(L"7", S5) CH_4 vs H_2 — which more prone to FB, to produce (more soot), which pollutants are we in H_2 vs CH_4?

Q13(L"7", S11) Why $T_{ad}[H_2] > T_{ad}[CH_4]$ @ peak?

Q14("7", S27) are probes accurate for cc?

Q15("7", S27) can we see the H_2 flame?

ANSWERS:

$\boxed{dh = \delta Q + Vdp}$ → isob. = 0. If isol V, then process must've been isochoric for the same

Q1. Q. energy balance en H not E/U ? so enthalpie/hardyc

Q1. @ $\phi=1$ what you have is max heat release (not temp)

Furthermore, @ $\phi=1$ you have maximum rate of dissociation which are endothermic, so steal that energy, which means @ $\phi=1$ the heat goes to the dissociation, not to increase T_{ad}. Lastly @ $\phi=1$ c_p is a bit higher than @ rich, so Temp can't be that high en the end.

2. At rich there's shortage of oxygen, so less dissociation

3. In rich mixtures the products include CO & H_2 which have lower c_p than fully oxidized products (CO_2 & H_2O)

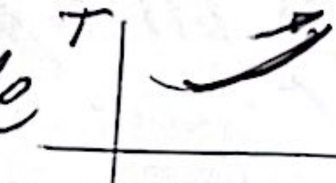
ALSO

4. @ $\phi=1$ products more fully oxidized but the energy release is partitioned into a) vibrational excitation of molecules (b) endoth. reactions) → duplikat

5. AD dissociation → less energy spent on bond breaking.

Q2. Higher, cuz 1st TD en isochoric no work so all heat into U (T↑)

Q3. Yes. T_{ad}↑ → more useful work available



But ∃ issues if T_{ad}↑. a) material tolerance, b) $T_{ad} \sim NO_x$ c) T↑ if @ $\phi > 1$, so leave out UHC & CO → η_{cc}↓

Q4. 1) Suppression of diss. @ high P (due to the Le Chatelier's principle — equilibrium shifts towards the side with less moles: $H_2O \underset{F}{\overset{D}{\rightleftharpoons}} \frac{1}{2}O_2 + H_2$ towards H_2O, so F ≡ formation where $\Delta H < 0$, so exothermic so T_{ad}↑.

2) "@ high P, the rr rate is enhanced which makes the combustion complete & release more en/per unit mole" CO (?)

Q5. The heat balance model assumes one-step, irrev, complete cc; adiabatic & isobaric sys; ∞ fast

Q what is missing? 1) Dissociation (endoth). 2) Minor radical species (carriers of h_f°); 3) pressure dependence ($p\uparrow \rightarrow$ diss$\downarrow$ — Le Chatelier $\rightarrow T_{ad}\uparrow$) 4) finite-rate chemistry & incomplete burn (other species c_p) 5) Heat loss, mixing (w colder streams), radiation $\longrightarrow$ so heat-balance-Tad is an upper bound!

Q: Note $G - F = H - U = PV > 0 \Rightarrow G > F$
So free en. > @ eqb rather than each.
Interestingly, $\Delta G = \Delta(pV) + \Delta F = \Delta F + RT\Delta n$
in combustion $\Delta n < 0$ usually, so
$\Delta G < \Delta F \rightarrow$ fall in gibbs is more -ve than in helm. So reaction is more favorable (spontaneous?) @ const pressure, not each.

Q6. Mean that change in gibbs for products is the same as for reactants $\rightarrow$ equilibrium. more tools equil

Q7.

Q8

Q9

Q10. @ higher p, dissociations are more suppressed, so $\gamma_{cc}\uparrow$. (@high p TIT$\uparrow$ so W$\uparrow$ but this is more of a compress effect, were talking about c here) Why they diverge? Recall for isentropic & isobaric: $Tds = \delta q = dh = c_p dT \Rightarrow \frac{dT}{ds} = \frac{T}{c_p}$
c_p grows with T but slower than T, so $T_s\uparrow \rightarrow$ diverge.

Q11 No.

Q13. No. time $\sim^{OOM} 10^{-3}$ [s], Δpace $\sim 10^{-4}$ [m]. Probes are these sizes.

Q14. No, H_2 flame emits OH* radicals @ $\approx$ 308 nm $\longrightarrow$ invisible (vis = 400–700]