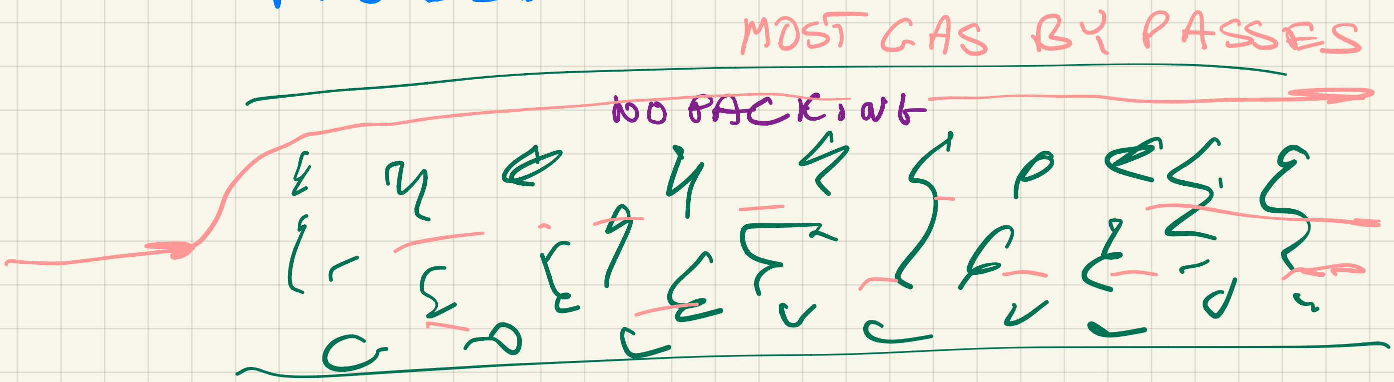
CBE 40445
TEST #3 REVIEW
CHAPTER 8, 9.

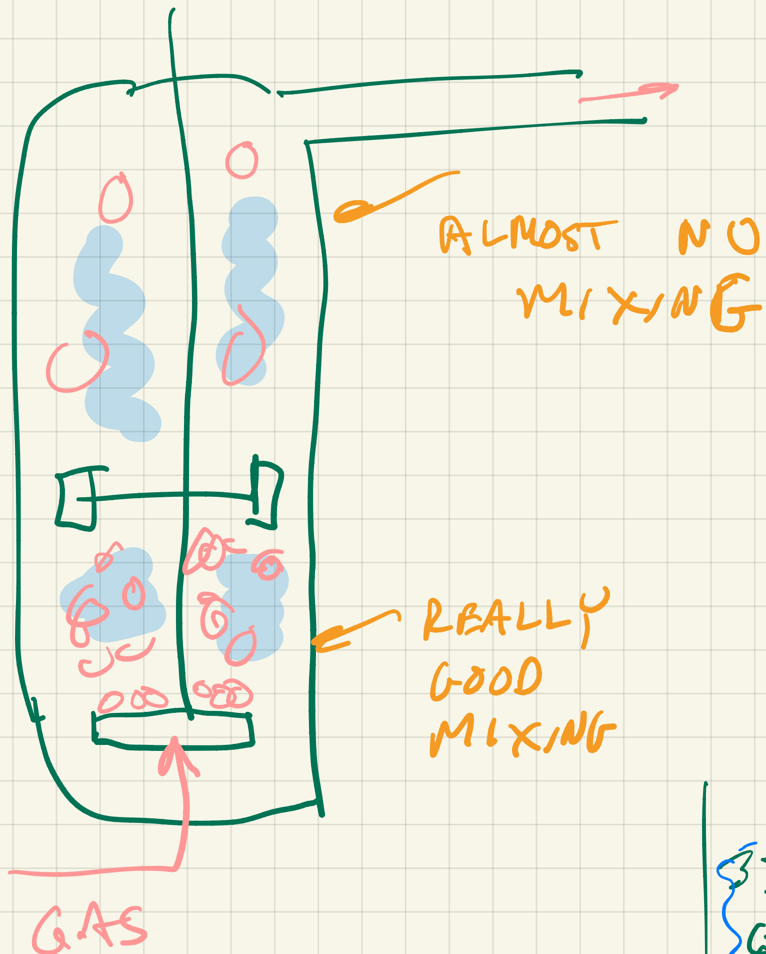
CHAPTER 8 NON IDEAL FLOW IN REACTORS

UNDERSTANDING THAT YOU SHOULD "BOLO" (BE ON LOOK OUT) FOR NONIDEALITIES.

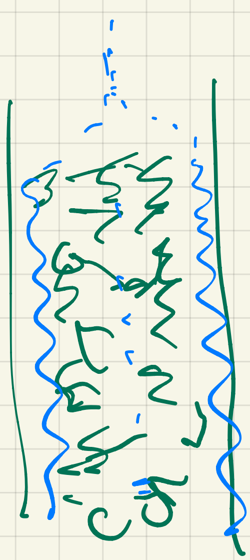
LOOKING OUT FOR THESE IS MORE IMPORTANT THAT KNOWING HOW TO SOLVE A SPECIFIC PROBLEM.

RATHER OVERT PHYSICAL PROBLEMS:

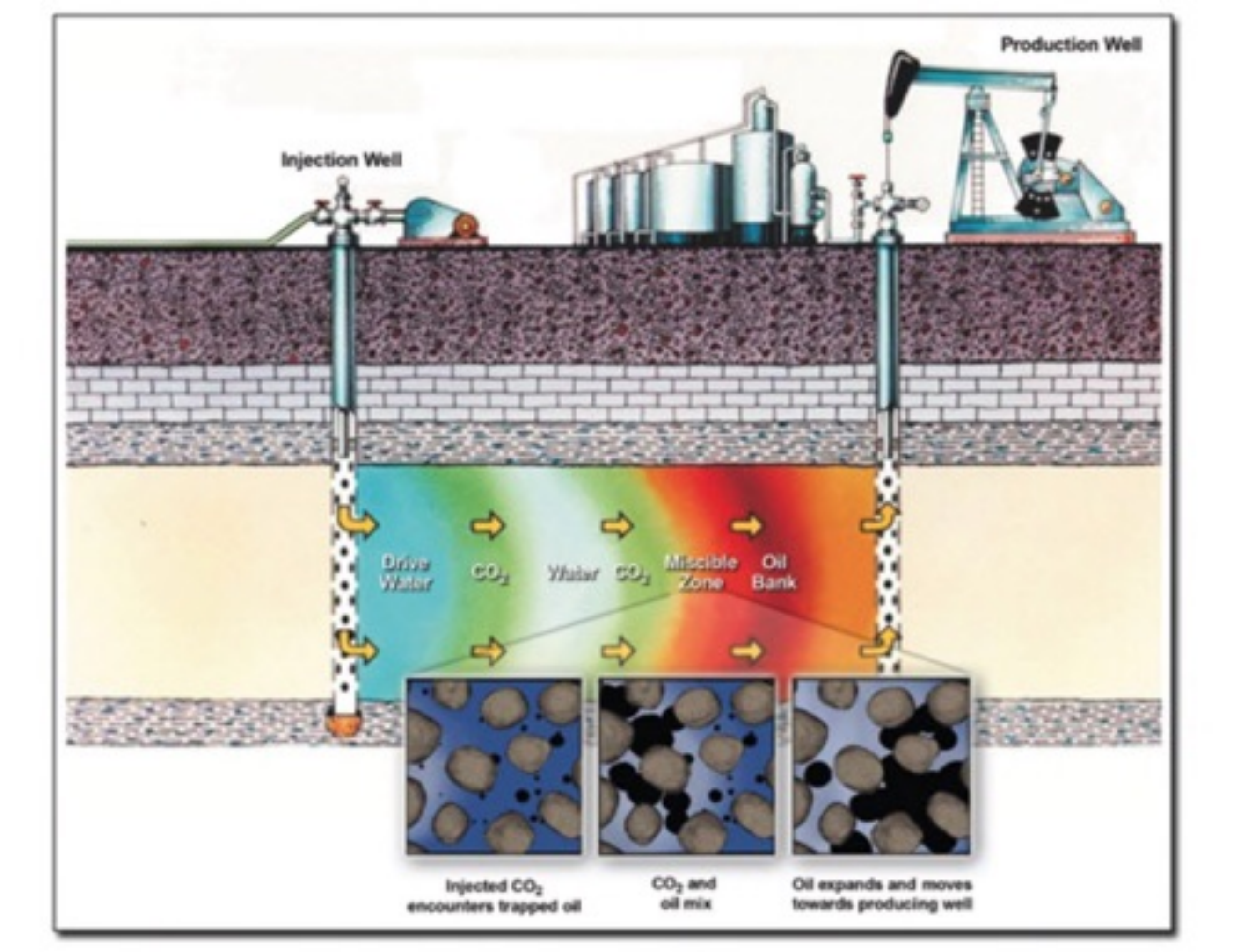




EFFORTS AT GETTING $\underset{\sim}{F_A}$ WILL BE THWARTED

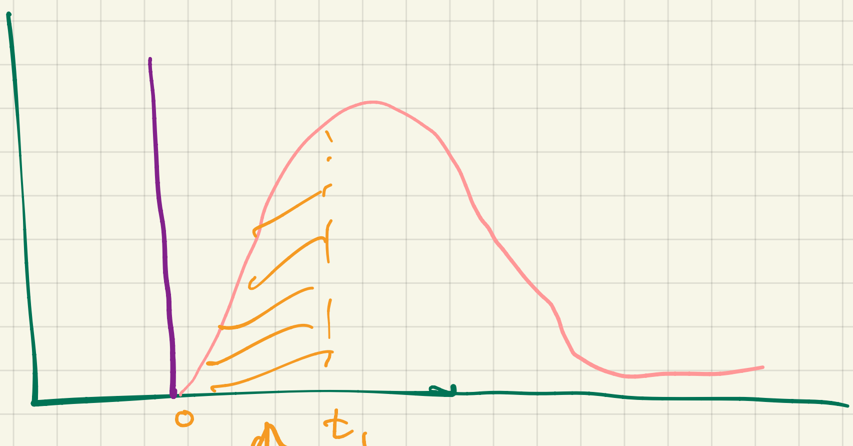


WATCH FOR LIQUID RUNNING DOWN WALLS


Production Well
Injection Well
Drive Water
CO_2
Water
CO_2
Miscible Zone
Oil Bank
Injected CO_2 encounters trapped oil
CO_2 and oil mix
Oil expands and moves towards producing well

WHAT IS IDEAL FOR CSTR!

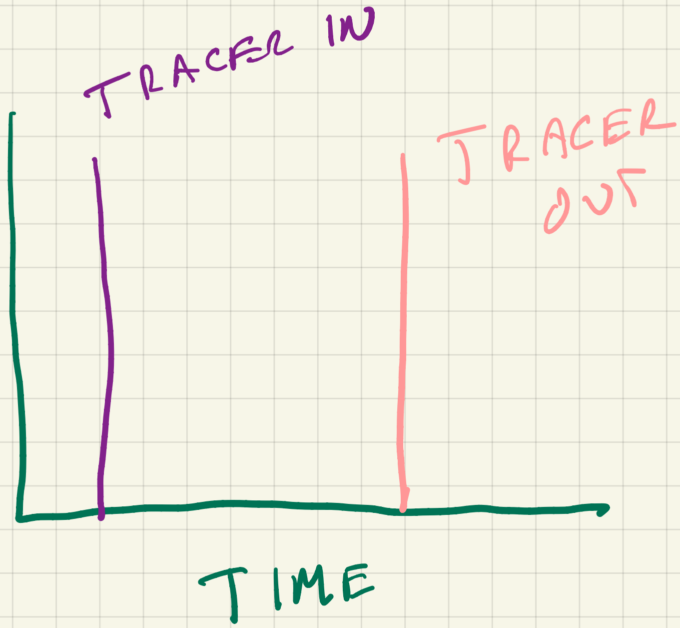
WHAT IS MORE LIKELY?

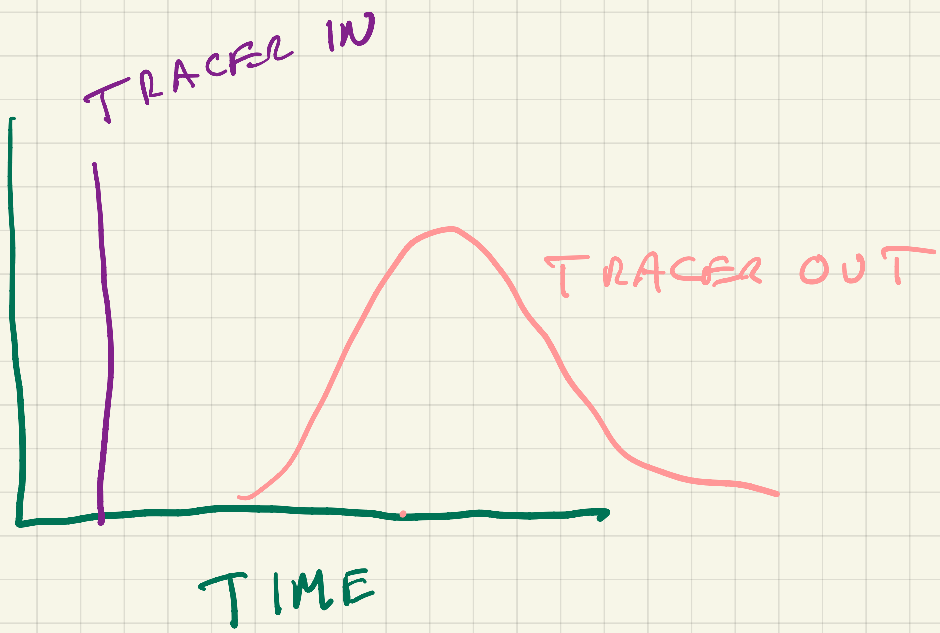


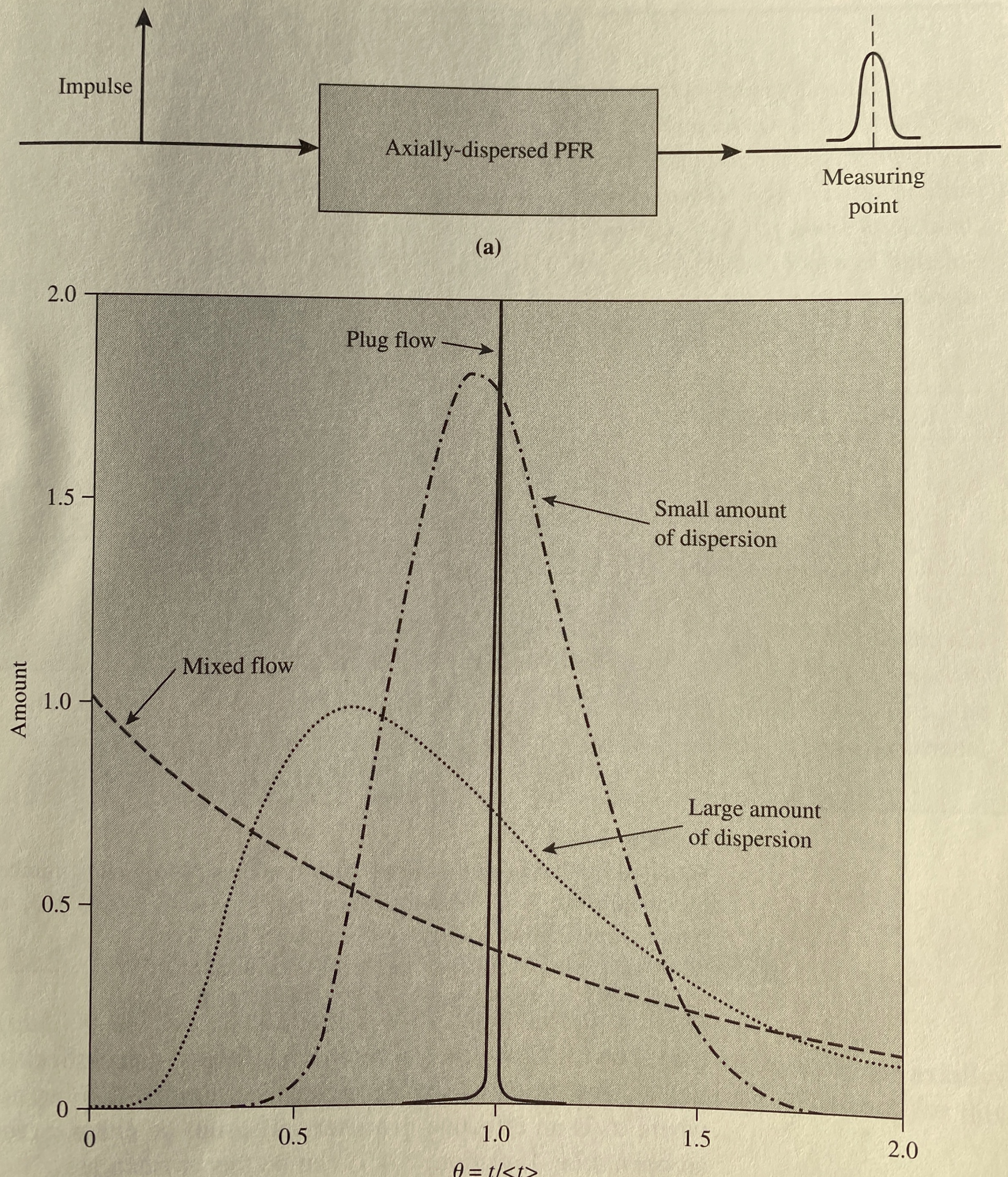
$$\int_0^{t_1} E(t)\,dt$$

$$E(t) = \frac{C_A(t)}{\int_0^{\infty} C_A(\bar{t})\,d\bar{t}}$$

WHAT IS IDEAL FOR A PFR!







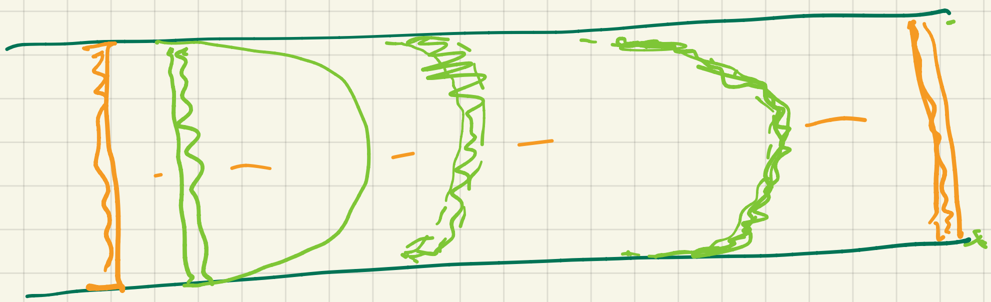
MOLECULAR DIFFUSION + FLOW INDUCED DISPERSION

$$\frac{\partial c}{\partial t} = D_A \frac{\partial^2 C}{\partial x^2}$$

$$u \frac{\partial c}{\partial x} = D_A \frac{\partial^2 c}{\partial x^2}$$

OPEN PIPE REACTOR

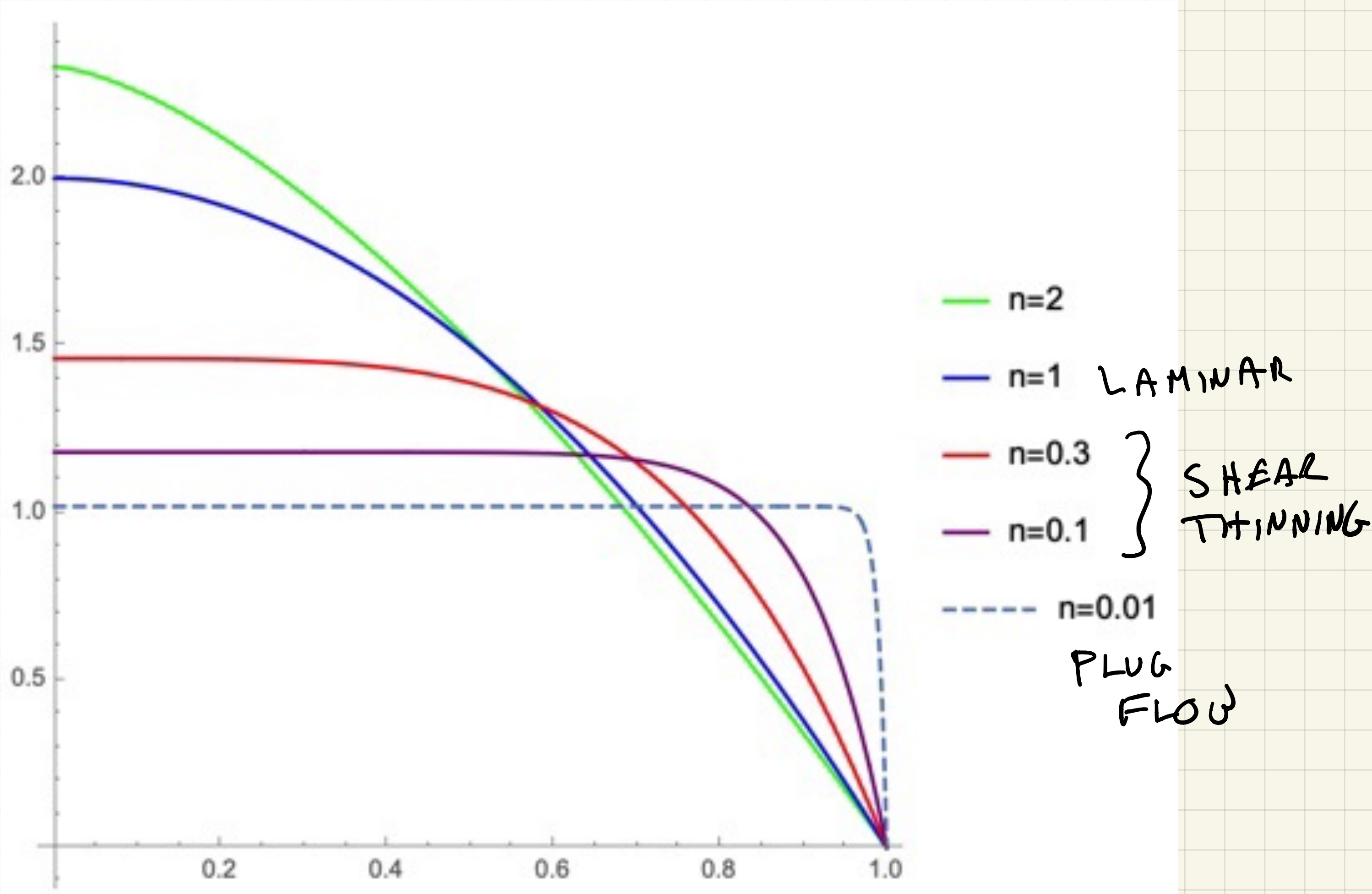
MIGHT OCCUR IN MICROFLUIDIC DEVICE



IF "PLUG FLOW" THEN

IF LAMINAR FLOW, CENTER OF PIPE WOULD EXIT FIRST

POWER-LAW VELOCITY PROFILES



$$u(r) = \frac{2^{-1/n}\, n \left(\frac{\mathrm{dpdz}}{K}\right)^{1/n} \left(R^{\frac{n+1}{n}} - r^{\frac{n+1}{n}}\right)}{n+1}$$

$$\bar{u} = \frac{2^{-1/n}\, n \left(R^{\frac{1}{n}+2} - \frac{n\, R^{\frac{1}{n}+2}}{2\, n+1}\right) \left(\frac{\mathrm{dpdz}}{K}\right)^{1/n}}{n+1}$$

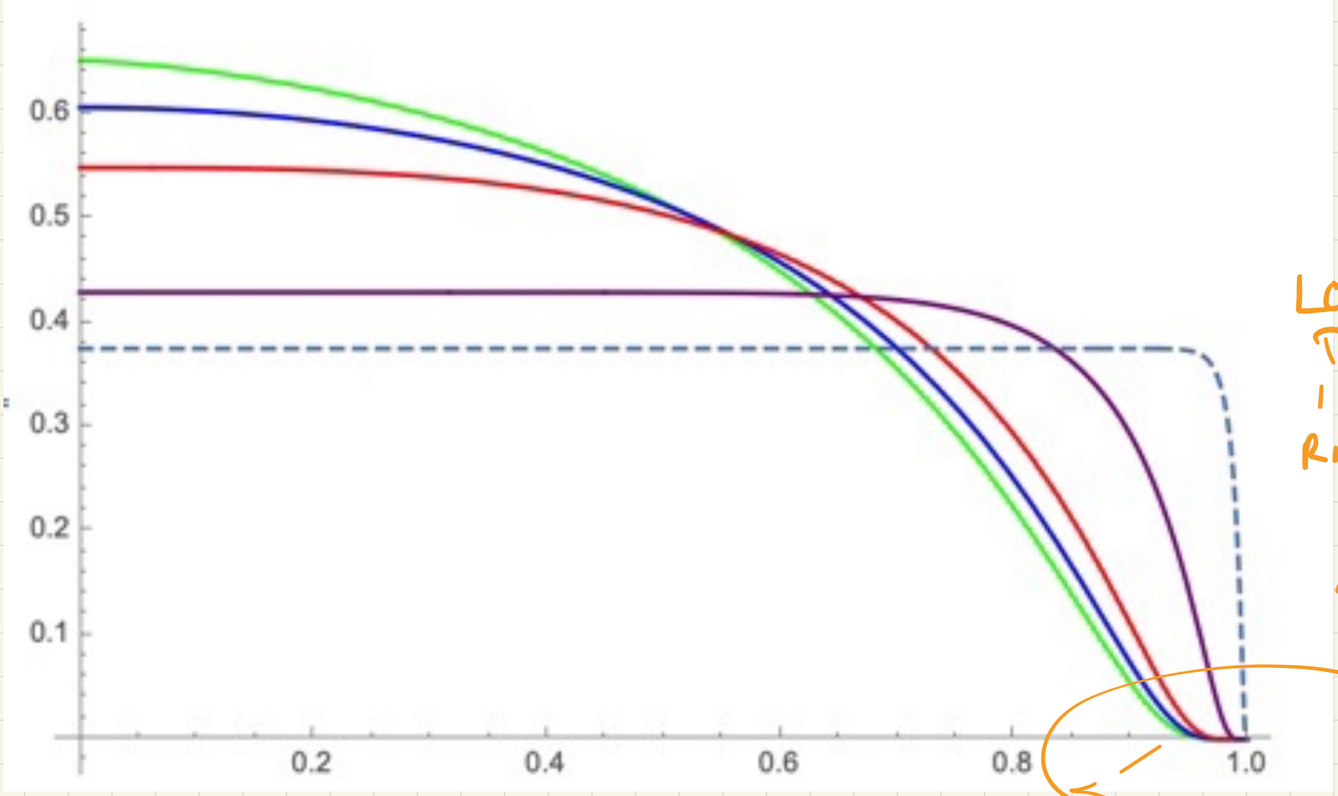
FOR $\tau = 1$, $k = 1$,

$\exp(-k\tau) = .368$

FOR FLOW REACTOR

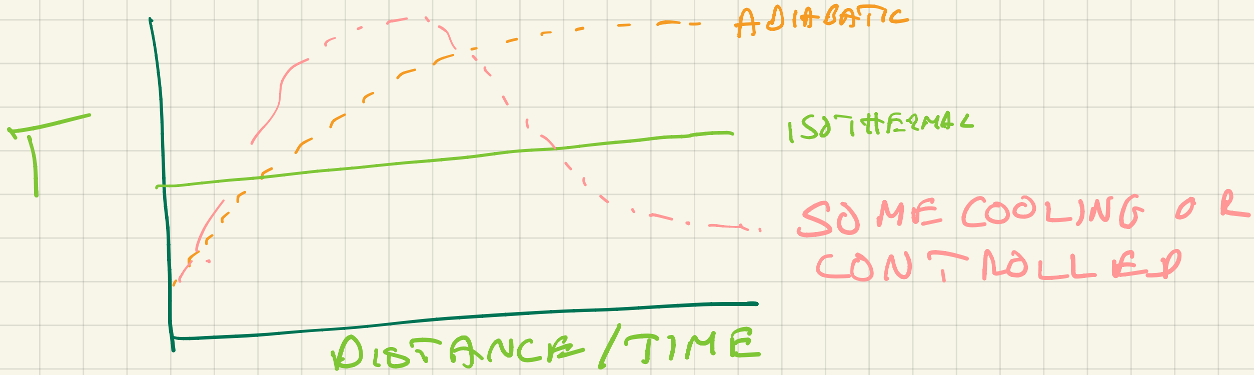
m	$\bar{C}_A^{EXIT}$
2	.453
1	.443
.5	.429
.3	.416
.1	.392
.01	.371

COULD BE A DIFFERENCE



LONG TIME IN REACTOR

NON ISOTHERMAL REACTORS . . .



added to the system and negative signs if energy is removed from the system.

The complete energy balance is as follows:

$$\frac{d}{dt}\left\{M\left(\hat{U}+\frac{v^2}{2}+gh\right)\right\}=\sum_{j=1}^{j=J}\left\{\dot{m}_{j,\text{in}}\left(\hat{U}_j+P_j\hat{V}_j+\frac{v_j^2}{2}+gh_j\right)\right\}$$
$$-\sum_{k=1}^{k=K}\left\{\dot{m}_{k,\text{out}}\left(\hat{U}_k+P_k\hat{V}_k+\frac{v_k^2}{2}+gh_k\right)\right\}+\dot{W}_S+\dot{W}_{EC}+\dot{Q} \qquad (3.33)$$

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The complete energy balance is as follows:

CONST V

$$\boxed{\frac{d}{dt}\left\{M\left(\hat{U}\right.\right.}+\cancel{\frac{v^2}{2}}^{\,0}+\cancel{gh}^{\,0}\Big)\Big\}=\sum_{j=1}^{j=J}\left\{\dot{m}_{j,\text{in}}\left(\underbrace{\hat{U}_j+P_j\hat{V}_j}_{\hat{H}}+\cancel{\frac{v_j^2}{2}}^{\,0}+\cancel{gh_j}^{\,0}\right)\right\}$$
$$-\sum_{k=1}^{k=K}\left\{\dot{m}_{k,\text{out}}\left(\underbrace{\hat{U}_k+P_k\hat{V}_k}_{\hat{H}}+\cancel{\frac{v_k^2}{2}}^{\,0}+\cancel{gh_k}^{\,0}\right)\right\}+\underbrace{\dot{W}_S}_{\text{USUALLY } 0}+\cancel{\dot{W}_{EC}}^{\,0}+\underbrace{\dot{Q}}_{\text{HEAT IN OR OUT}} \qquad (3.33)$$

BATCH OR UNSTEADY STATE FLOW REACTOR

USUALLY 0

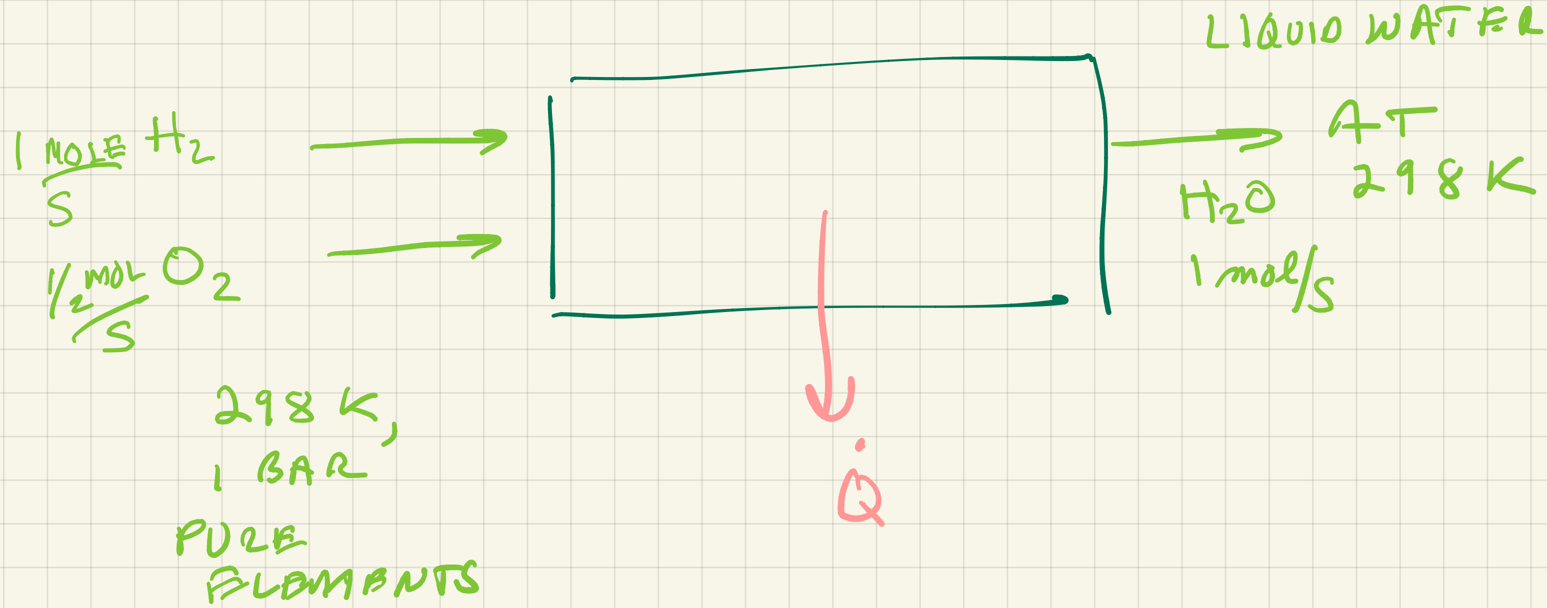
HEAT IN OR OUT

USUAL EQ FOR ENERGY!

S.S:
$$\dot{Q}=\dot{m}_{OUT}\,h_{OUT}-\dot{m}_{IN}\,h_{IN}$$

$$h_i\equiv\hat{H}_i \qquad \frac{\text{ENTHALPY}}{\text{MASS}}$$

HEAT OF REACTION / COMBUSTION



$$0 = \dot{m}_{H_2}\hat{H}_{H_2} + \dot{m}_{O_2}\hat{H}_{O_2} - \dot{m}_{H_2O}\hat{H}_{H_2O} + \dot{Q}$$

$$0 = (1)(0) + (1/2)(0) - (1\ mol/s)(285.8)\frac{kJ}{MOLE} + \dot{Q}$$

ENTHALPY OF FORMATION

$$\dot{Q} = -285.8\ \frac{kJ}{s}$$

THUS IF $CH_4 + 3O_2 \rightarrow CO_2 + 2H_2O$

$(-74.9) + 0 \qquad 393.5\ \frac{kJ}{MOLE} + 2(285\ kJ/MOLE)$

$$\dot{Q} = -888.6\ kJ/MOLE$$

BATCH REACTOR

$$\int_0^t UA_H (T^* - T)\,dt = \frac{-\Delta H_r\, r_{r_0}}{\nu_e}\, n_e^0 f_e + \sum_i \left(n_i \int_{T_{INITIAL}}^{T_{FINAL}} C_{p_i}\, dT \right)$$

A MORE CONVENIENT FORM:

$$UA_H (T^* - T) = \Delta H_r\, r V + \sum n_i C_{p_i} \frac{dT}{dt}$$

HEAT REMOVED BY EXTERNAL SINK

HEAT GENERATION FROM REACTION

HEAT NEEDED TO INCREASE T

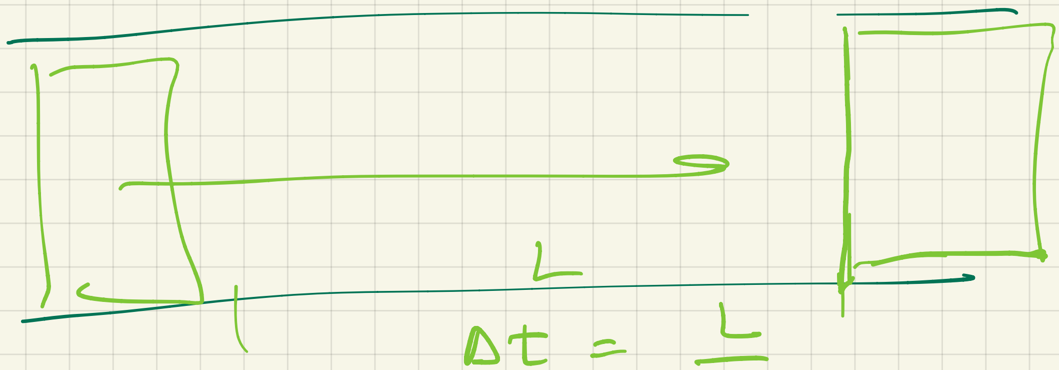
- FOR A TEST, COULD HAVE A SITUATION WHERE COOLING KEEPS T CONST

  → ? HOW MUCH COOLING ?

- COULD HAVE A SITUATION WHERE ΔT IS SMALL ..

  → NOT A BIG EFFECT ON RATE. , SOME FIXED COOLING.

PLUG FLOW REACTOR



$$\Delta t = \frac{L}{u}$$

SAME BEHAVIOR AS A

BATCH REACTOR

$$d\dot{Q} = -\frac{\Delta H_r}{V_\ell} F_\ell^0 \, df_\ell + \sum_i F_i^{OUT} \int_{T^0}^{T^{OUT}} c_{p_i} \, dT$$

$$- \sum F_i^{IN} \int_{T^0}^{T^{IN}} c_{p_i} \, dT$$

ADIABATIC

$$\sum F_i \int_{T^0}^{T} c_{p_i} \, dT = \frac{\Delta H_r}{V_\ell} F_\ell^0 \, df_\ell$$

PICK INLET T

$A \rightarrow M$

$$F_A^0 (1 - f_A)\, C_{pA} (T^{OUT} - T^{IN}) + F_A^0 f_A\, C_{pM} (T^{OUT} - T^{IN})$$

$$= \frac{\Delta H_r}{(-1)} F_A^0 f_A$$

IF f_A IS SPECIFIED, SOLVE FOR T.

TEMPERATURE EFFECTS IN A CSTR

HEAT REMOVAL = HEAT GENERATED − HEAT TAKEN UP BY COMPONENTS

$$\dot{Q} = \frac{F_\ell^{\circ}\left(\Delta H_r\big|_{T_0}\right)\overbrace{\left(f_\ell^{f} - f_\ell^{\circ}\right)}^{(-)}}{\underbrace{(-\nu_\ell)}_{(+)}} + \sum F_i^{f} \int_{T^0}^{T^f} c_p \, dT$$

FOR A → M CONST c_p

$\boxed{f_A^{\circ} = 0}$

$$0 = F_A^{\circ}(1 - f_A) - k C_A^{\circ}(1 - f_A) V$$

$$\dot{Q} = \underbrace{F_A^{\circ} \Delta H_r f_A}_{(-)} + \underbrace{F_A^{\circ} c_p (T - T^0)}_{+} + \underbrace{F_N c_p (T - T_0)}_{+}$$

F_N ↑ INERTS

IF $\dot{Q} = 0$, AND f IS SPECIFIED, THEN EQ CAN BE SOLVED FOR T

COULD ALSO ASK,

WHAT IS $\dot{Q}$ IF REACTOR IS ISOTHERMAL?

→ SOLVE ISOTHERMAL CASE

$\rightarrow V$

$$\dot{Q} = \Delta H_r k C_A V$$

$$\dot{Q} = \Delta H_r F_A^0 f_A$$

$$UA(T^* - T) = \Delta H_r k C_A V$$

$(-)$

COOLING SO $T^* < T$