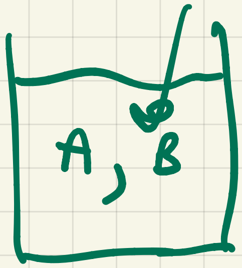
CBE 40455

8/26/20

REVIEW

BATCH REACTOR



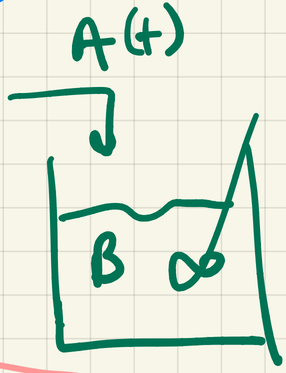
$$\frac{dm_i}{dt} = \nu_i r V$$

$A + B \rightarrow 2M$

$$\frac{dC_A}{dt} = -kC_AC_B$$

$$\frac{dC_B}{dt} = -kC_AC_B$$

SEMI BATCH



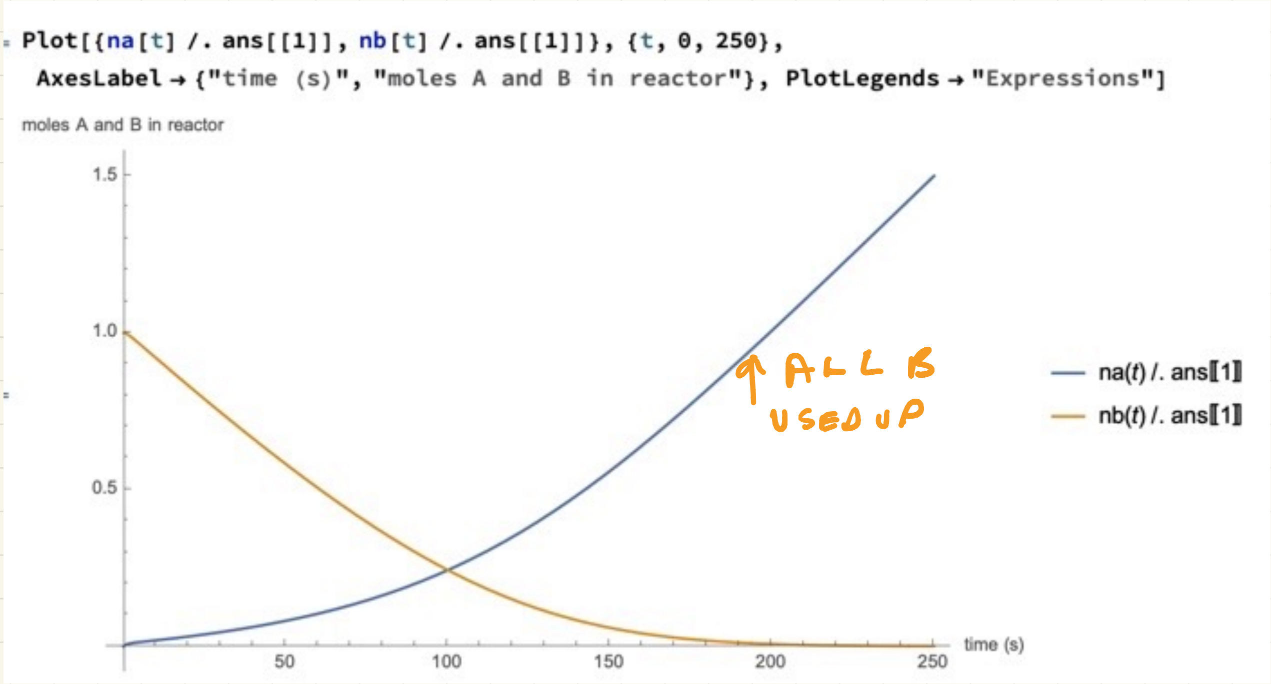
FEED COULD BE CONTROLLED OR VARIED BY RECIPE.

$T = T(t)$

$$\frac{dm_A}{dt} = q(t)\,C_A^0 + \nu_i r V$$

$$\frac{dm_B}{dt} = \qquad + \nu_i r V$$

SOLVE NUMERICALLY



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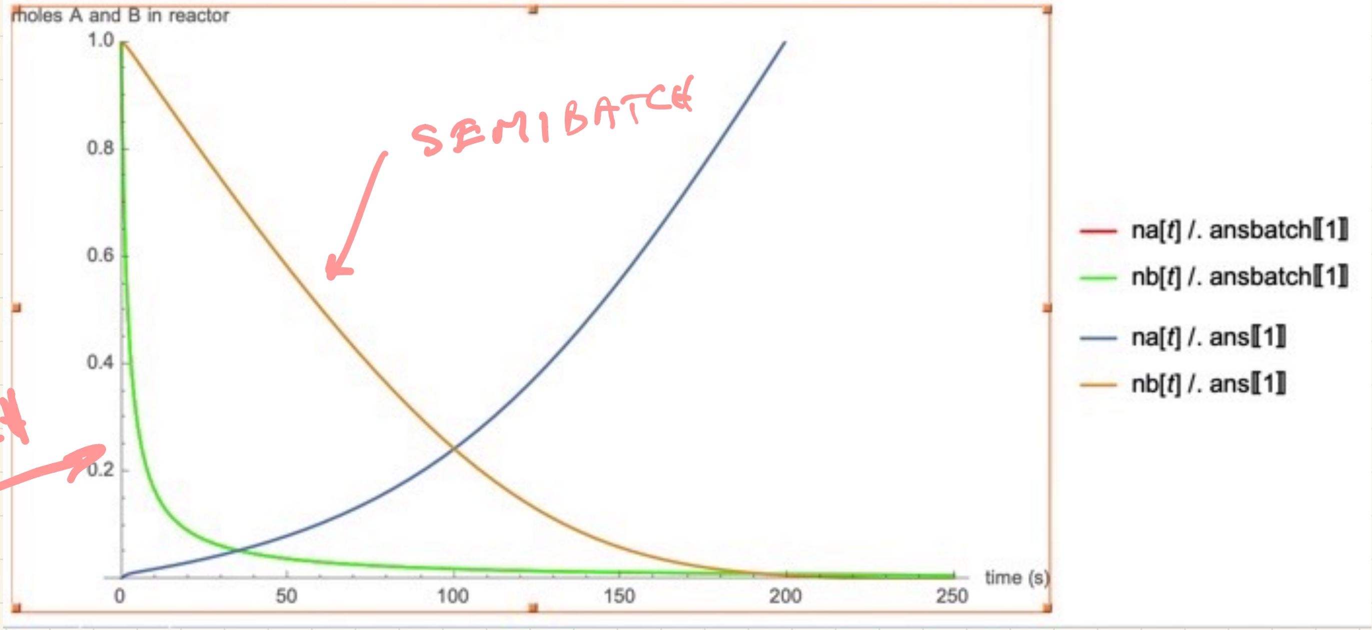
Plot[{na[t] /. ans[[1]], nb[t] /. ans[[1]]}, {t, 0, 250},
 AxesLabel → {"time (s)", "moles A and B in reactor"}, PlotLegends → "Expressions"]
```

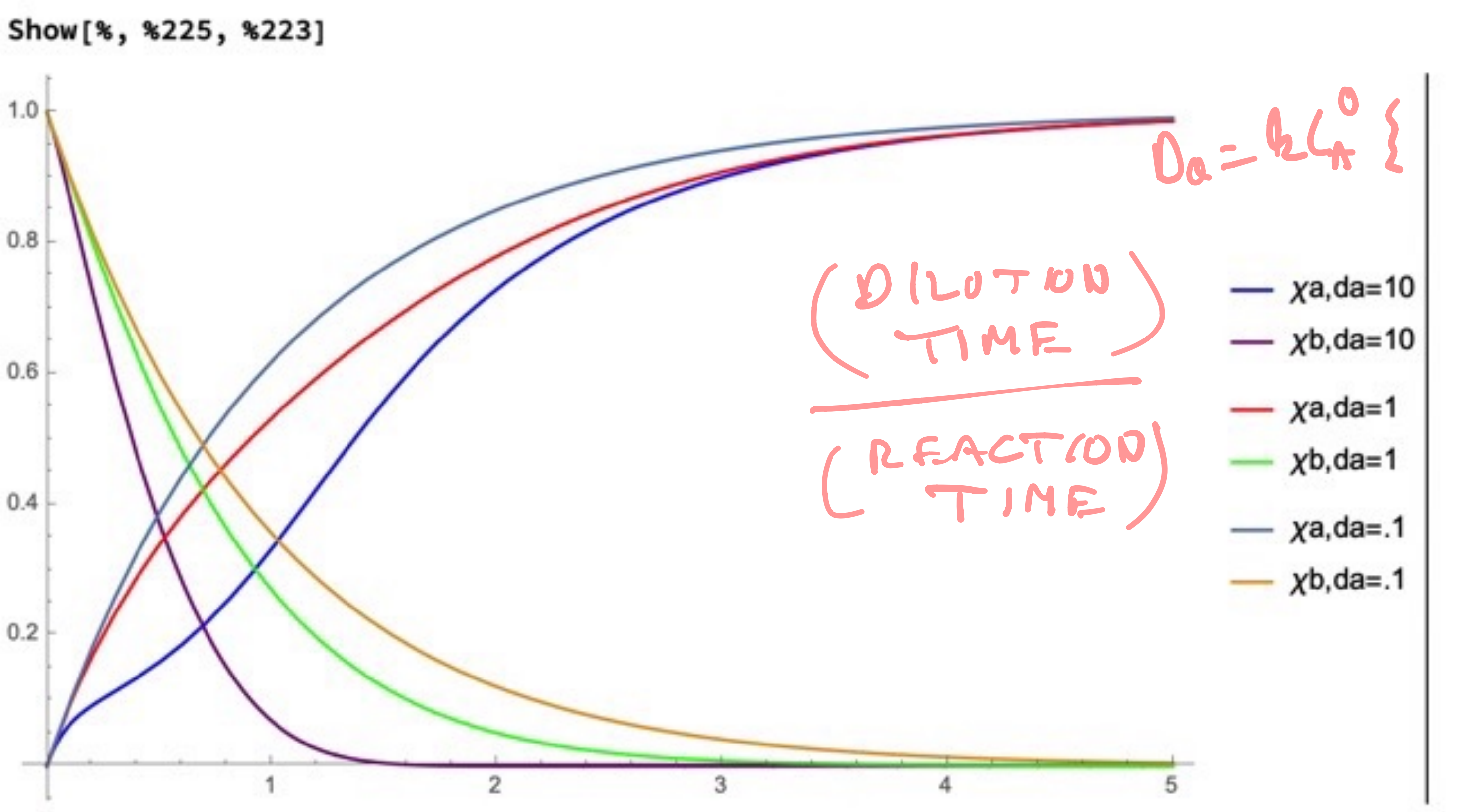
↑ ALL B USED UP

IF ALL A IS ADDED AT BEGINNING, REACTION IS MUCH FASTER



SEMIBATCH

BATCH



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Show[%, %225, %223]
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$Da = k C_A^0 \tau$

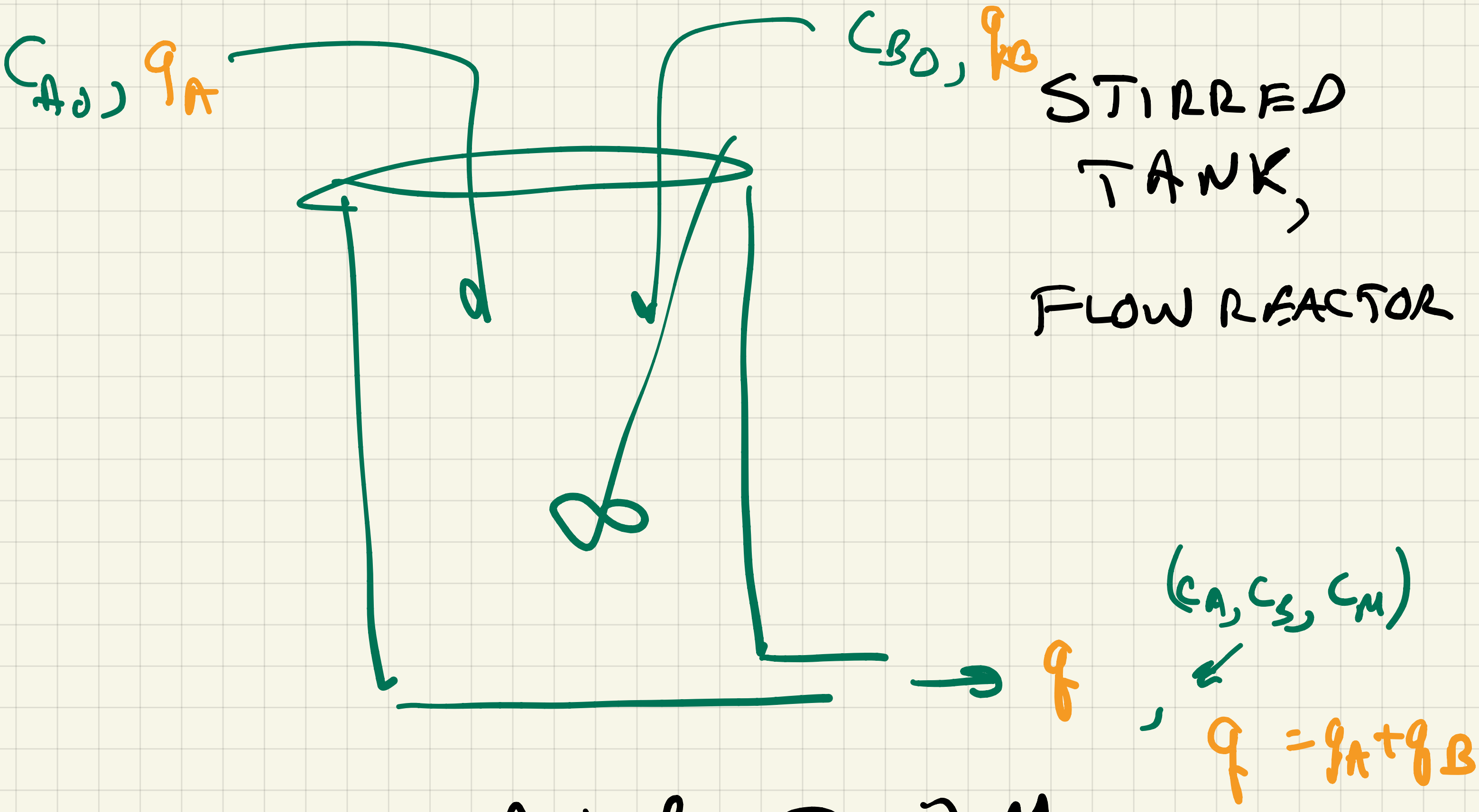
$$Da = \frac{(\text{DILUTION TIME})}{(\text{REACTION TIME})}$$

$$\left\{ \begin{aligned} \frac{d x_A}{d\tau} &= (1 - x_A) - Da\, x_A x_B \\ \frac{d x_B}{d\tau} &= -x_B - Da\, x_A x_B \end{aligned} \right.$$

AS Da ↑ FASTER REACTION

BUT THIS IS MITIGATED SOME WHAT BY "A" GETTING USED UP

CONTINUOUS FLOW STIRRED TANK REACTOR "CSTR"



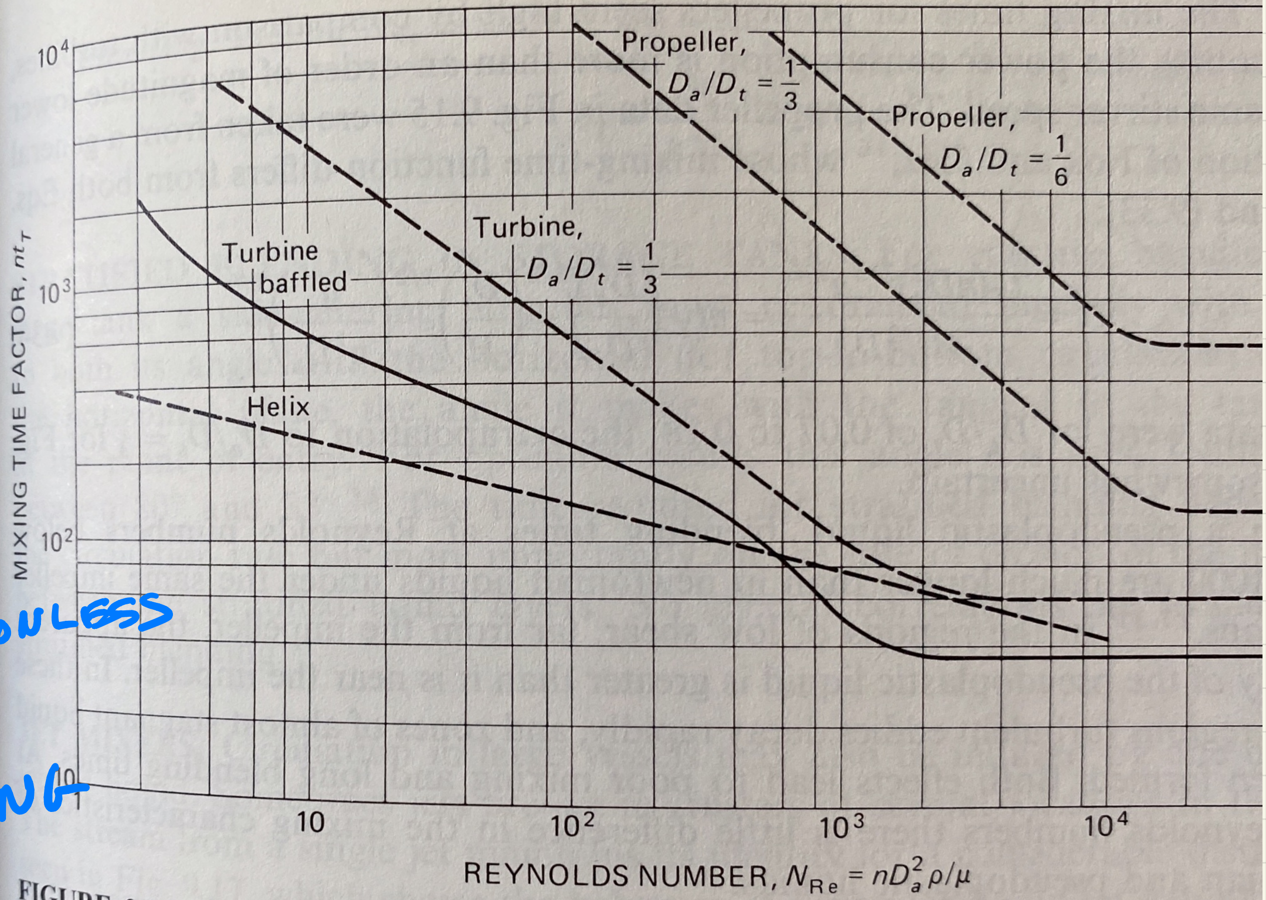
$$A + B \rightarrow 2M$$

THIS OPERATES AT EXIT COMPOSITION. C_A, C_B

THUS TO GET GOOD CONVERSION OF A + B, VOLUME NEEDS TO BE MUCH LARGER, THAN A BATCH REACTOR

$$r = k C_A C_B$$

"TYPICAL" AGITATION CURVE FOR A STIRRED TANK

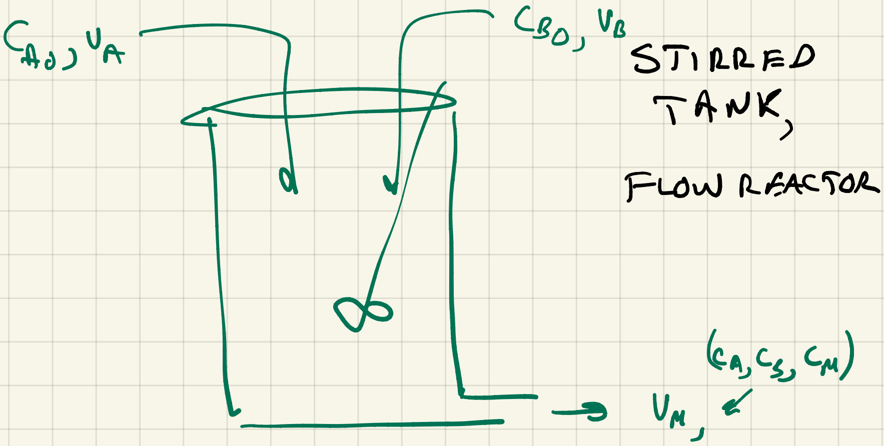


DIMENSIONLESS TIME OF MIXING

FIGURE 9.15
Mixing times in agitated vessels. Dashed lines are for unbaffled tanks; solid line is for an unbaffl

IMELLER ROTATION FREQUENCY

NEED TIME SCALE FOR MIXING < REACTION TIME SCALE



$$A + B \rightarrow 2M$$

GENERAL EQUATIONS!

OVERALL MASS BALANCE

$$\frac{d\rho V}{dt} = \rho_A q_A + \rho_B q_B - \rho q$$

CHANGE IN DENSITY IS NOT AN ISSUE FOR LIQUIDS IF NO ΔV_{mix}

$$\frac{dV}{dt} = q_A + q_B - q$$

(COULD BE FILLING UP.)

$$\frac{dm_A}{dt} = F_A^0 - F_A + r_A V$$

COMPONENT A $$\frac{d}{dt} V C_A = q_A C_{A0} - q C_A + \nu_A r V$$

COMPONENT B $$\frac{d}{dt} V C_B = q_B C_{B0} - q C_B + \nu_B r V$$

COMPONENT M $$\frac{d}{dt} V C_M = 0 - q C_M + \nu_M r V$$

STANDARD ASSUMPTIONS FOR STEADY-STATE OPERATION.

$$\frac{d}{dt}(\ ) = 0$$

JUST LOOK AT COMPONENT A. → $A + B \rightarrow 2M$

$$0 = q_A C_{A0} - q C_A + \nu_A r V$$

$$C_A = \frac{q_A C_{A0}}{q} + \nu_A r \frac{V}{q}$$

OR

$$-\nu_A r = \frac{q_A C_{A0} - q C_A}{V}$$

WE CAN WRITE:

$$-\nu_A r = \frac{F_{A0} - F_A}{V}$$

$\frac{\text{MOLES}}{\text{TIME}}$

WE COULD ALSO WRITE:

$$f = \frac{F_{A0} - F_A}{F_{A0}}$$

WHICH GIVES:

$$-\nu_A r = \underbrace{\frac{F_{A0}}{V} f_A}$$

$k C_A^2$

MOST USEFUL FOR LIMITING REACTANT.

COULD BE A GOOD FORM FOR MEASURING KINETICS

WHAT IS "TIME SCALE" FOR A CSTR OPERATING AT STEADY STATE?

f, C_A, V, q, k

ACTUALLY THIS COULD BE THOUGHT OF AS A "TRICK" QUESTION

- REACTION TIME SCALE

$$\frac{1}{k} , \quad \frac{1}{kC_A^0}$$

- FLOW TIME SCALE

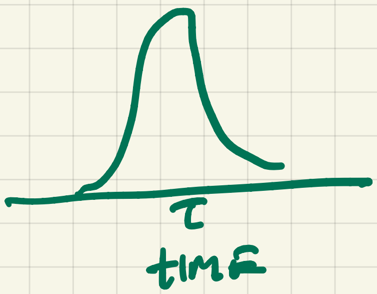
$$\tau \equiv \frac{V}{q} =$$ "SPACE TIME"

OR

"RESIDENCE TIME"

<u>AVERAGE</u> AMOUNT OF TIME A PACKET OF FLUID STAYS IN REACTOR

THERE WILL BE A DISTRIBUTION



WE CAN COMPARE TIME OF REACTION FOR A BATCH REACTOR TO τ FOR A CSTR

$$A \rightarrow M$$

BATCH

$$\frac{dC_A}{dt} = -kC_A \qquad C_A(0) = C_{A0}$$

$$\ln \frac{C_A}{C_{A0}} = kt$$

$$\frac{C_A}{C_{A0}} = \exp(-kt)$$

EXPONENTIAL DECAY

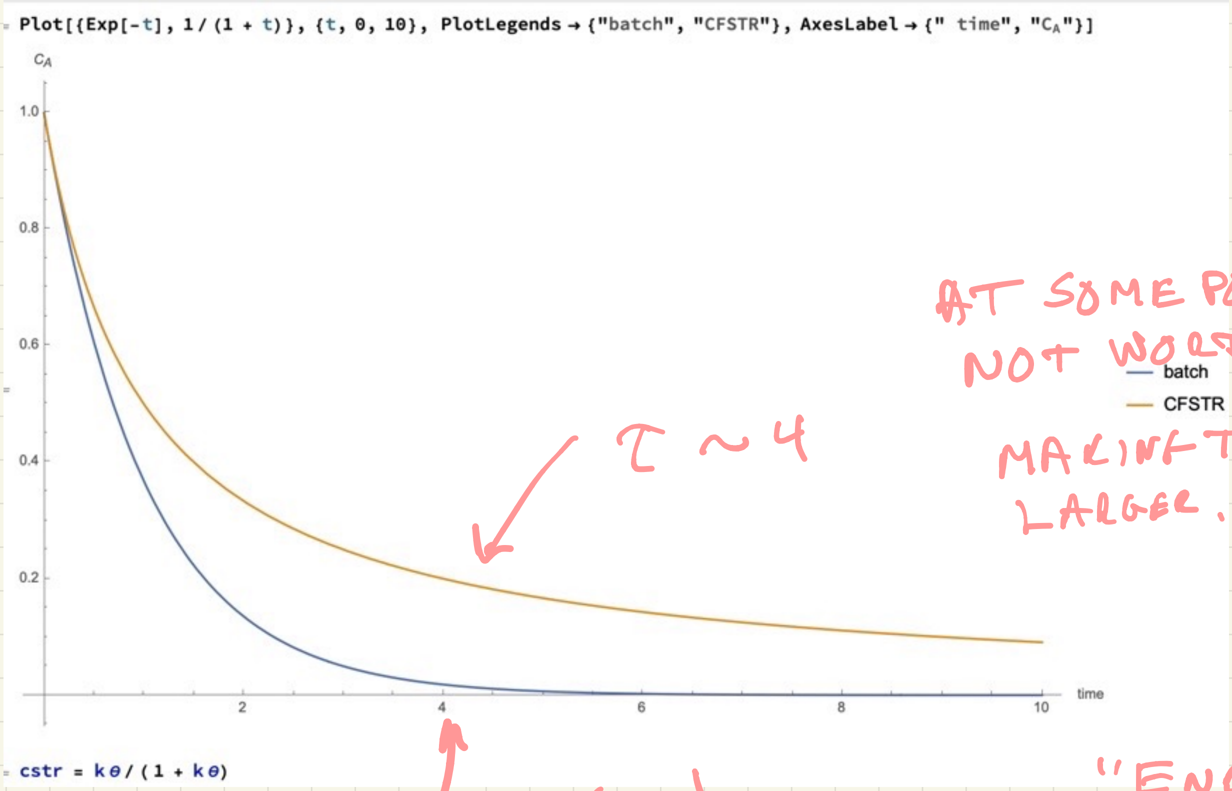
CSTR

$$0 = qC_{A0} - qC_A - kC_A V$$

$$0 = q - q\frac{C_A}{C_{A0}} - k\frac{C_A}{C_{A0}} V$$

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + k\frac{V}{q}} = \frac{1}{1 + k\tau}$$

ALGEBRAIC DECAY



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Plot[{Exp[-t], 1/(1 + t)}, {t, 0, 10}, PlotLegends → {"batch", "CFSTR"}, AxesLabel → {" time", "CA"}]
```

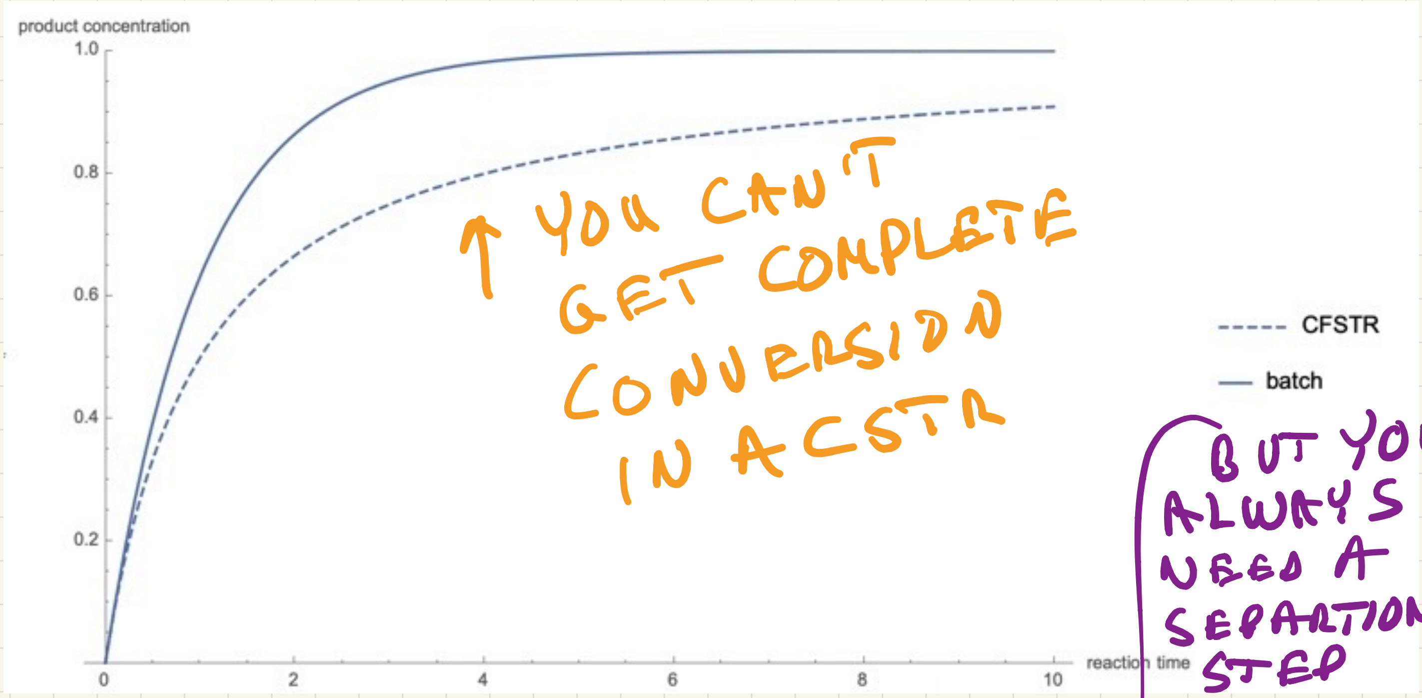
```
cstr = k θ / (1 + k θ)
```

AT SOME POINT NOT WORTH MAKING THIS LARGER...

$\tau \sim 4$

$\exp(-4) < .02$

"END" FOR A 1ST ORDER CHANGE PROCESS.



↑ YOU CAN'T GET COMPLETE CONVERSION IN A CSTR

BUT YOU ALWAYS NEED A SEPARTION STEP ANYWAY!!

KINETICS FROM CSTR

1ST ORDER

$$k = \frac{C_{A0} - C_A}{C_A \ \tau}$$

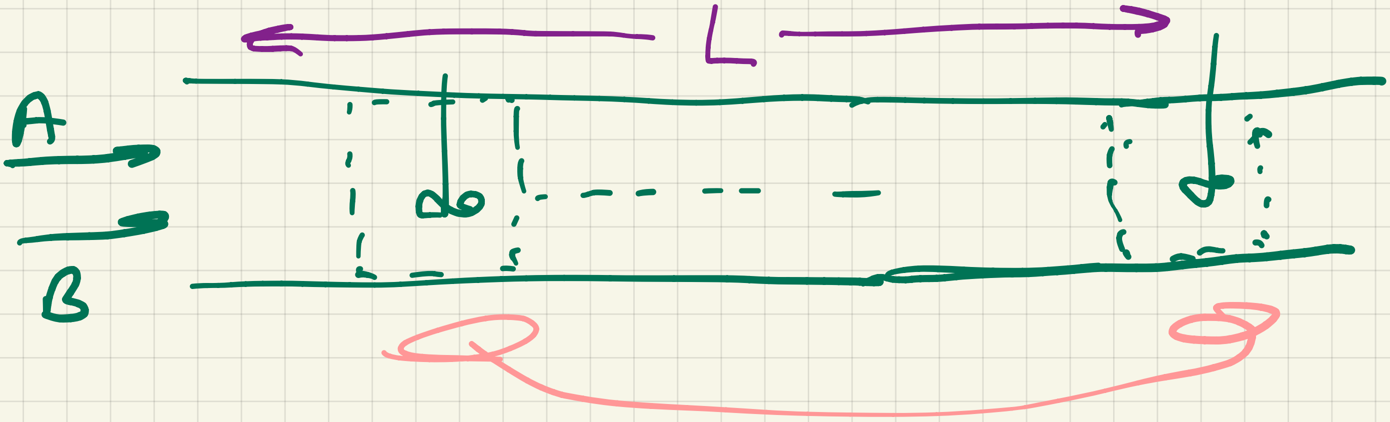
2ND ORDER

$$k C_A C_B = \frac{C_{A0} - C_A}{\tau}$$

$$k = \frac{C_{A0} - C_A}{\tau \ C_A C_B}$$

JUST NEED GOOD STEADY STATE CONCENTRATION MEASUREMENTS

TUBULAR REACTORS



SAME FLUID

"PLUG FLOW"

FOLLOWING THIS SCENARIO A "PFR" (PLUG FLOW REACTOR) IS THE SAME AS BATCH:

$$t \rightarrow \frac{\overbrace{L A_c}^{\text{VOLUME}}}{\underset{\uparrow\ \text{VOLUMETRIC FLOW RATE}}{q}} = \tau$$

UTILITY OF TUBULAR REACTORS

1) SOLID CATALYST THAT CAN OPERATE AS A PACKED BED

AS OPPOSED TO A "SLURRY" INSIDE A TANK

→ TIME PERIOD IN OPERATION

→ TIME PERIOD FOR REGENERATION

2) HIGHLY EXOTHERMIC REACTIONS

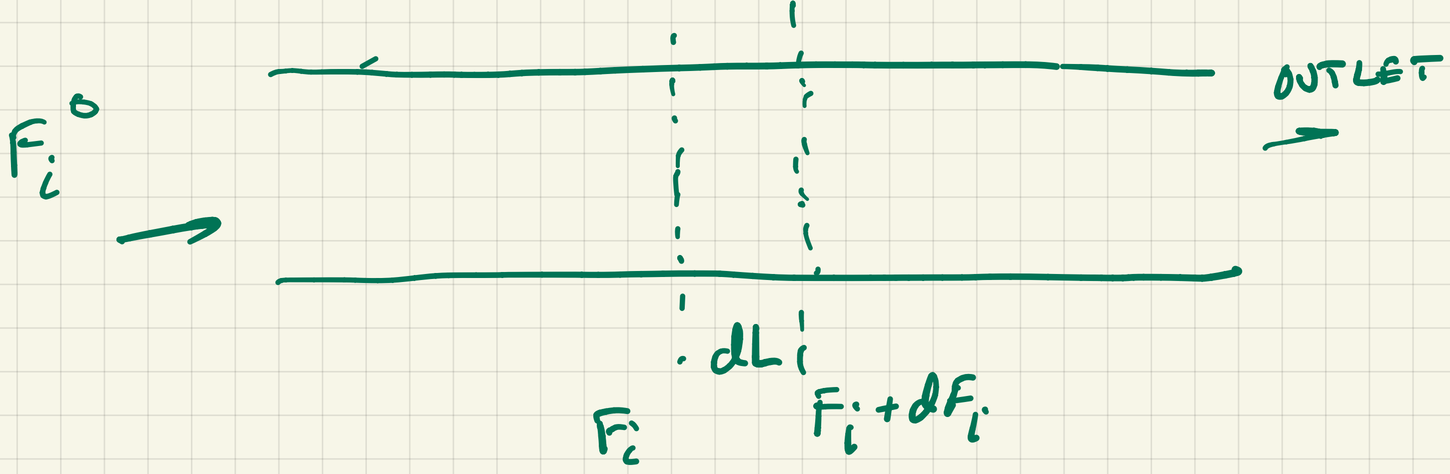
COOLING AROUND "EACH" TUBE

→ SHELL + TUBE HEAT EXCHANGER

3) CONTINUOUS FLOW + HIGH CONVERSION

PFR ANALYSIS

STEADY OPERATION



FOR DIFFERENTIAL SLICE:

$$0 = \underbrace{F_i}_{\text{MOLAR FLOW IN}} - \underbrace{(F_i + dF_i)}_{\text{MOLAR FLOW OUT}} + \underbrace{\nu_i r A_c dL}_{\text{MOLES REACTED}}$$

$$\frac{1}{A_c}\frac{dF_i}{dL} = \nu_i r$$

$$F_i = q C_i$$

$$\tau = \frac{V}{q} = \frac{L A_c}{q}$$

$$d\tau = \frac{A_c}{q} dL$$

$$\frac{q}{A_c}\frac{dC_i}{dL} = \underbrace{\frac{dC_i}{d\tau} = \nu_i r}_{\text{SAME AS BATCH REACTOR}}$$

$$\frac{dC_i}{d\tau} = \nu_i r$$

IF $r = k C_A$

$$\frac{dC_A}{d\tau} = -k C_A$$

THEN:

$$\ln \frac{C_A}{C_{A0}} = k\tau = k \frac{V}{q}$$

MORE GENERALLY

$$\frac{1}{A_c} \frac{dF_i}{dL} = \nu_i r$$

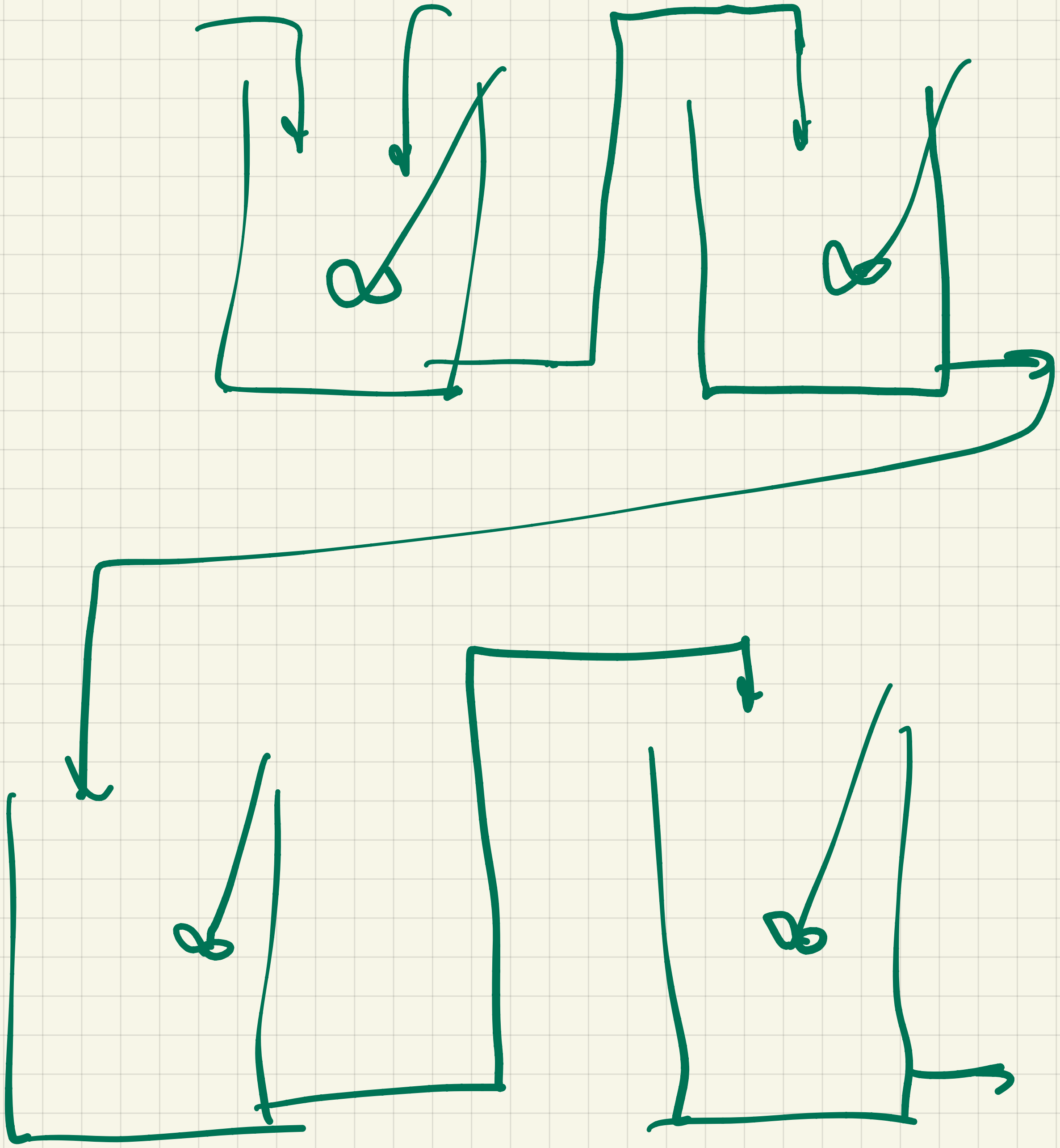
$$\frac{F_i^0}{A_c} \frac{df_i}{dL} = -\nu_i r$$

$$\frac{A_c L}{F_i^0} = \frac{V_R}{F_i^0} = \int_{f_i^0}^{f_i^{\text{OUTLET}}} \frac{df_i}{\nu_i r}$$

OR:

$$\tau = \frac{V_R}{q} = C_i^0 \int_{f_i^0}^{f_i^{\text{OUTLET}}} \frac{df_i}{\nu_i r}$$

IF CSTR CONVERSION
IS NOT SUFFICIENT
PUT MULTIPLE ONES
IN SERIES...



FIRST ORDER REACTION

$$\frac{C_A^1}{C_{A0}} = \frac{1}{1+k\tau}$$

$$\frac{C_A^2}{C_A^1} = \frac{1}{1+k\tau}$$

$$\frac{C_A^3}{C_A^2} = \frac{1}{1+k\tau}$$

$$\therefore \quad \frac{C_A^4}{C_{A0}} = \frac{1}{(1+k\tau)^4}$$

$$\frac{C_A^N}{C_{A0}} = \frac{1}{\left(1+\frac{k\tau^T}{N}\right)^N}$$

$$\frac{C_A^N}{C_A^0} = \frac{1}{\left(1+\frac{k\tau^T}{N}\right)^N} \cong \frac{1}{\text{Exp}(k\tau^T)}$$

$$\frac{C_A^\infty}{C_A^0} = \exp(-k\tau^T)$$

For $k = 1$, $\tau = 1$

N	$\frac{C_A^N}{C_A}$	$\frac{C_A^\infty}{C_A}$
1	.5	
2	.44	
3	.42	
4	.4096	
5	.402	.368
6	.397	

ONLY DO

~ 4