CBE 40445

8/28/20

- TEST ON 9/4
  - CHAPTS 1–3
    IF "COVID" ONLY TOPICS DIRECTLY RELATED TO MASS BALANCE, REACTIONS ETC.

- CSTR

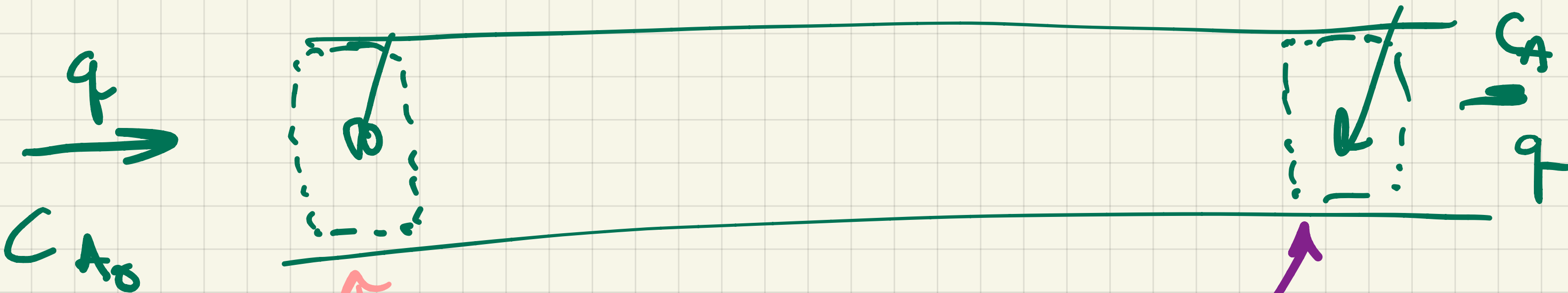
$$A \rightarrow M$$

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

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

- SPACE TIME
- RESIDENCE TIME

"PLUG FLOW" REACTORS



WELL MIXED ONLY LOCALLY

WHAT HAPPENS FOR LAMINAR FLOW?

PACKET OF FLUID IS IN REACTOR OF VOLUME V

FOR TIME =

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

THUS τ IS EQUIVALENT TO t FOR A BATCH REACTOR

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

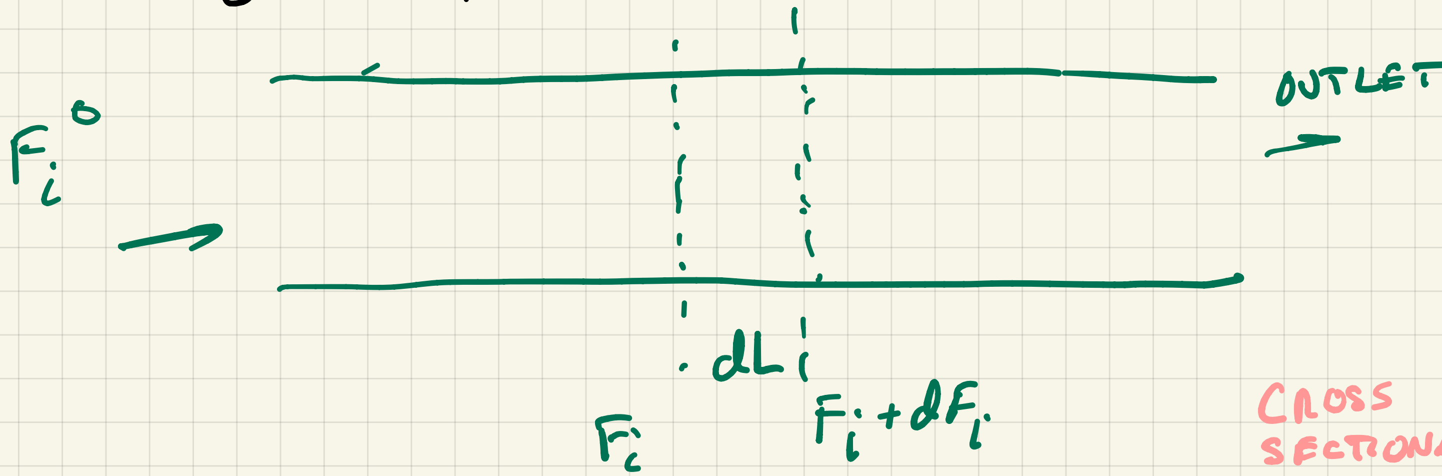
COOLING AROUND "EACH" TUBE

→ SHELL + TUBE HEAT EXCHANGER

3) CONTINUOUS FLOW + HIGH CONVERSION

PFR ANALYSIS

STEADY OPERATION



FOR DIFFERENTIAL SLICE:

CROSS SECTIONAL AREA

$$0 = F_i - (F_i + dF_i) + \nu_i r A_c dL$$

MOLAR FLOW IN

MOLAR FLOW OUT

MOLES REACTED

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

$$F_i = q C_i$$

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

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

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

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

IF $r = k C_A$

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

THEN:

$$\ln \frac{C_A}{C_{A_0}} = -k\tau = -k \frac{V}{q}$$

MORE GENERALLY

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

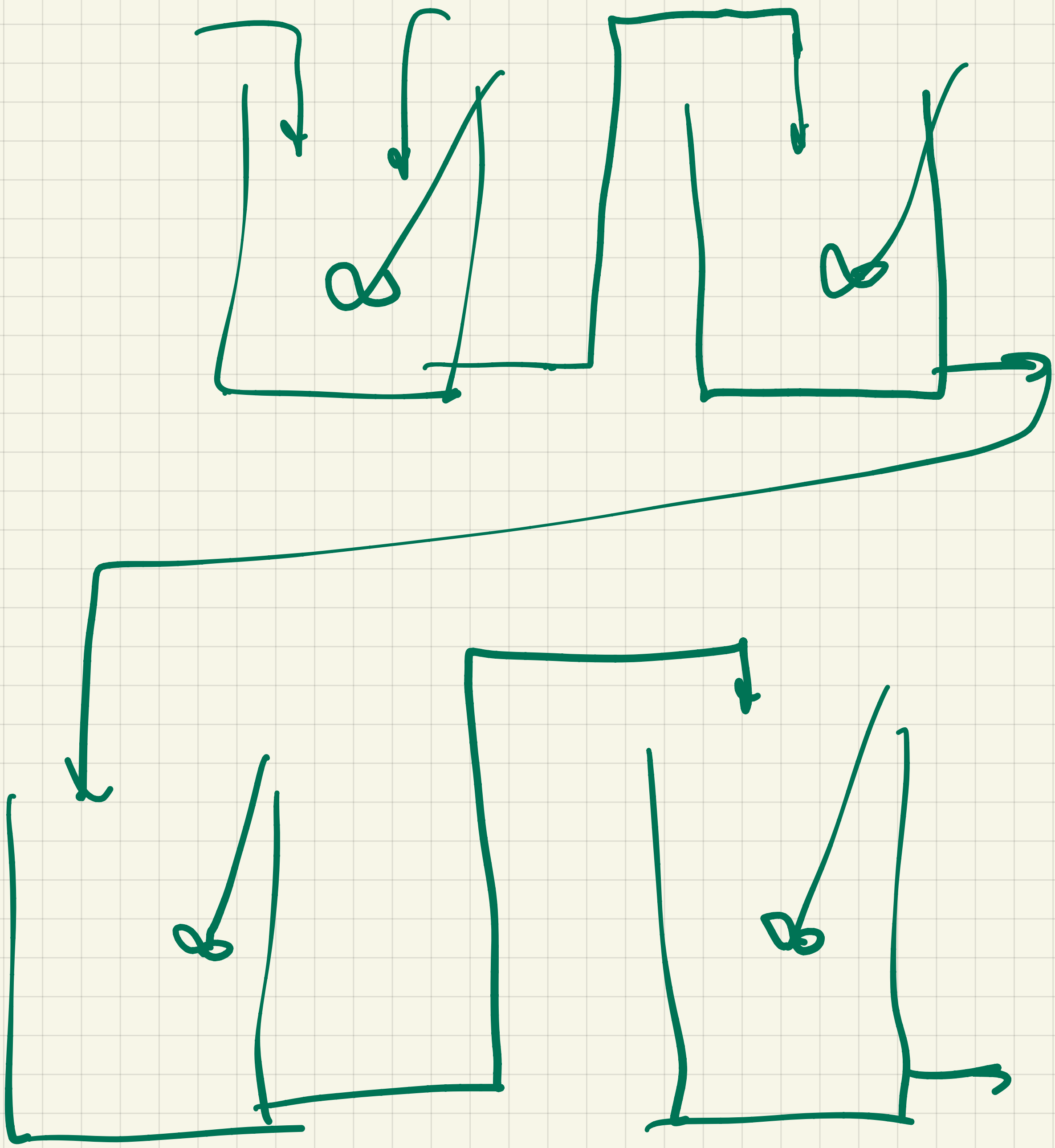
$$\frac{F_i^0}{A_c} \frac{df_i}{dL} = -\nu_i r$$

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

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

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

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

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

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

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

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

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

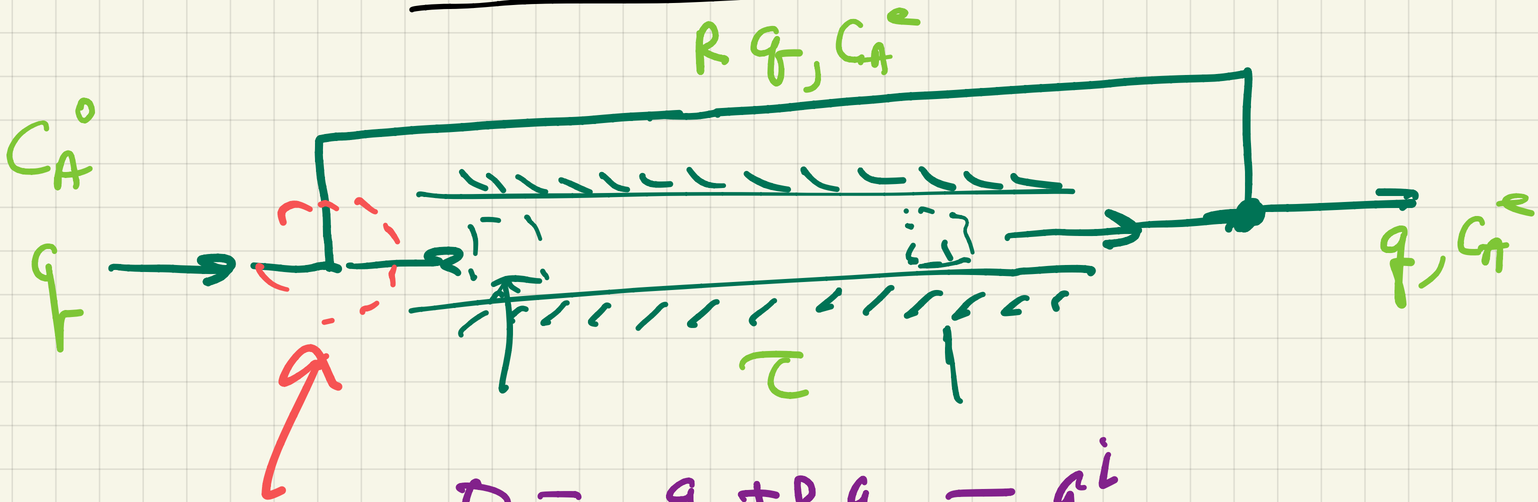
For $k=1$, $\tau=1$

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

USE OF RECYCLE



$$0 = q + Rq - q^i$$
$$q^i = (R+1) q$$

FOR REACTION: $\tau = \dfrac{V}{q(R+1)}$

$$0 = C_A^0 q + C_A^e R q - (R+1) q C_A^i$$

$$C_A^i = \frac{C_A^0 + R C_A^e}{R+1}$$

WE WILL CONTINUE ON BUT

IF $R = 0$ $\quad C_A^i = C_A^0$

AS $R \to \infty$ $\quad C_A^i = C_A^e$??

CONSIDER 1ST ORDER KINETICS:

COMPONENT MASS BALANCE ON REACTOR

RATE CHANGE OF MOLES OF A WITH PROGRESS THROUGH REACTOR = RATE OF REACTION IN REACTOR

$$\frac{dF_A}{dV_R} = \nu_A r$$

$$\frac{d\,qC_A}{A_c\,dL} = -kC_A$$

$$(1+R)q\frac{dC_A}{A_c\,dL} = -kC_A$$

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

$$(1+R)\frac{dC_A}{d\tau} = -kC_A$$

$$\frac{dC_A}{C_A} = -\frac{1}{R+1}k\,d\tau$$

$$\int_{C_A^i}^{C_A^e} \frac{dC_A}{C_A} = -\frac{1}{R+1} k \, d\tau$$

$$\ln \frac{C_A^e}{C_{A_i}} = -\frac{1}{R+1} k \tau$$

- WE WILL CHOOSE R.

- $$C_A^i = \frac{C_A^o + R C_A^e}{R+1}$$

- $$\tau = \frac{V}{q(R+1)}$$

$$\ln\left(\frac{C_A^e}{\frac{C_A^o + R C_A^e}{R+1}} \right) = -\frac{1}{R+1} k \frac{V}{q(R+1)}$$

$$C_A^e = -\frac{C_A^0(1+R)}{R^2 + R - \exp\left(\frac{kV}{q(1+R)^2}\right)}$$

WE CAN PLOT THIS AS A FUNCTION OF R

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Plot[%12 /. {ca0 → 1, k → .1, V → 10, q → 1}, {rr, 0, 10}, AxesLabel → {"R", "CAe/Ca0"}]
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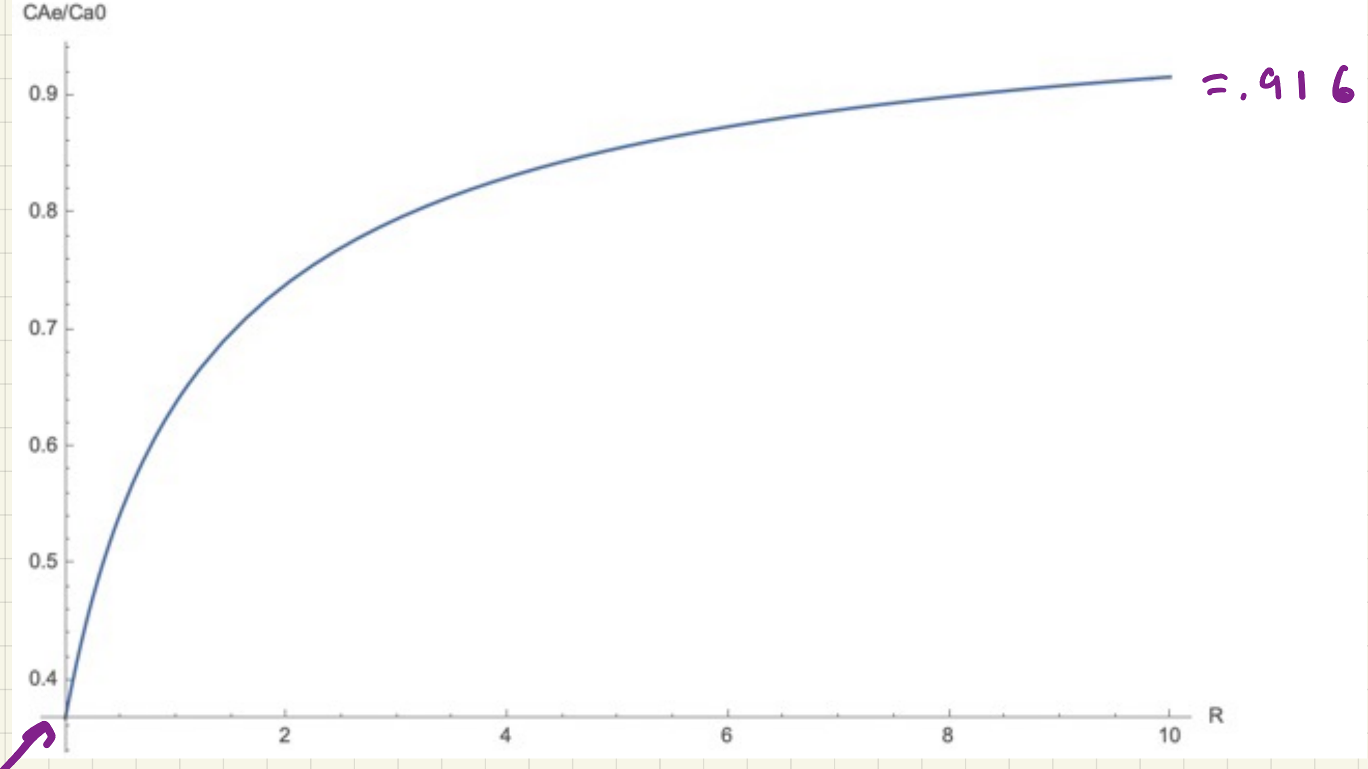

$= .916$

IF NO RECYCLE

$$\frac{C_A^0}{C_{A0}} = \exp(-k\tau)$$

$$= \exp(-1) = .367$$

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Plot[%12 /. {ca0 → 1, k → 1, V → 10, q → 1}, {rr, 0, 20}, AxesLabel → {"R", "CAe/Ca0"}]
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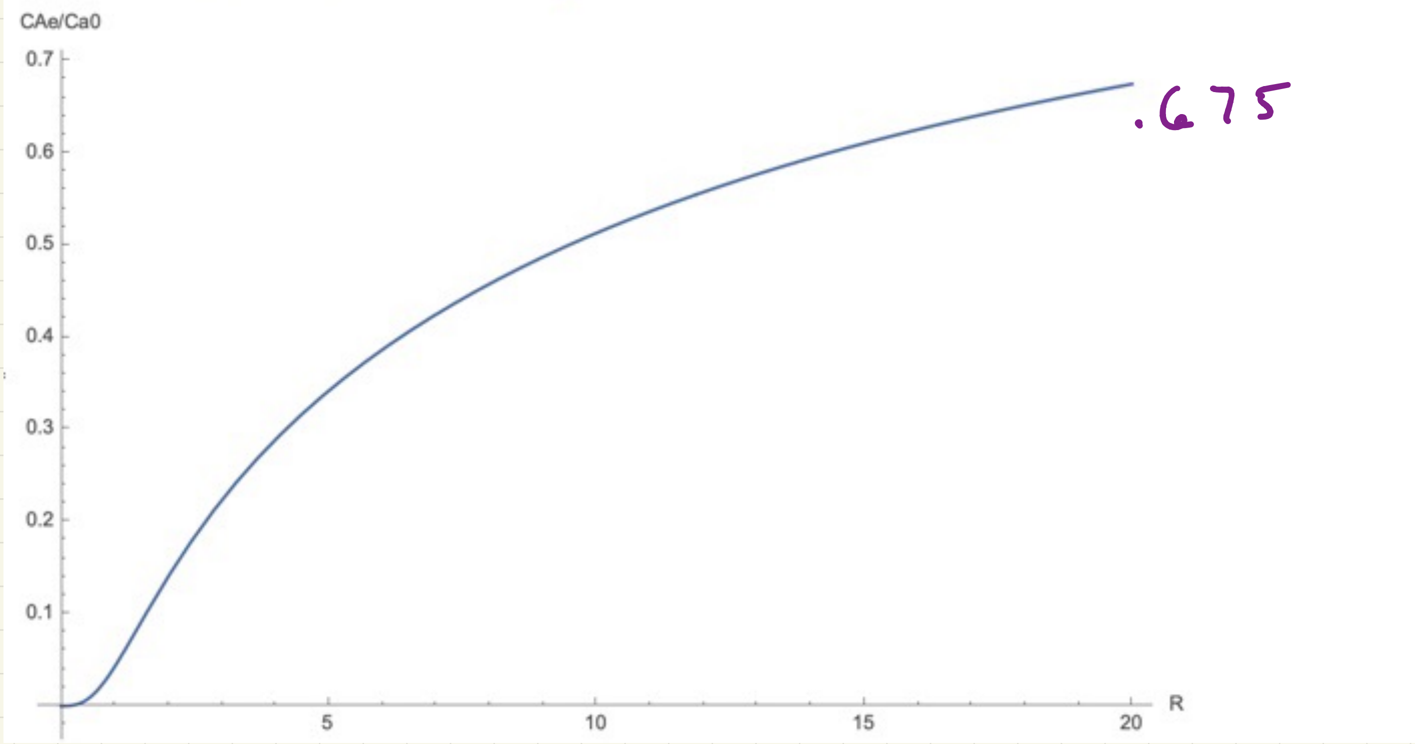


BATCH $\quad \dfrac{C_A}{C_{A_0}} = \exp(-10) \sim 4\times10^{-5}$

CSTR $\quad \dfrac{C_A}{C_A} = \dfrac{1}{1+\frac{1}{2}} = .667$

RECALL FOR CSTR

$$\frac{C_A}{C_A^0} = \frac{1}{1+k\tau}$$

$$= \frac{1}{1+(.1)\frac{10}{(R+1)1}}$$

$$= .91677 \qquad R=10$$

LOOKS LIKE RECYCLE REACTOR IS APPROACHING CSTR!

"BACK MIX REACTOR"

$$\ln\left(\frac{C_A^e}{\frac{C_A^0 + R\,C_A^e}{R+1}}\right)$$

$$\frac{C_A^e\,(R+1)}{C_A^0 + R\,C_A^e}$$

$$\frac{C_A^e\left(1+\frac{1}{R}\right)}{\frac{C_A^0}{R} + C_A^e}$$

$\varepsilon = \frac{1}{R}$

$$\ln\left(1 + \frac{C_{Ae} - C_A^0}{C_{Ae}}\,\varepsilon\right) \rightarrow \ln(1+x) \simeq x$$

$$\simeq \frac{C_A^e - C_A^0}{C_A^e}$$

$$\left(1 - \frac{C_A^0}{C_A^e}\right)\frac{1}{R} \simeq -\frac{kV}{qR^2}$$

$$-\frac{1}{R+1}\,k\,\frac{V}{q(R+1)}$$

$$-\frac{kV}{q}\,\frac{1}{(R+1)^2}$$

$R >> 1$

$$-\frac{kV}{qR^2}$$

$$\left(1 - \frac{C_A^0}{C_A^e}\right)\frac{1}{R} \cong -\frac{kV}{qR^2}$$

$$\frac{C_A^0}{C_{Ac}} = 1 + \frac{kV}{qR}$$

LOOKS LIKE CSTR

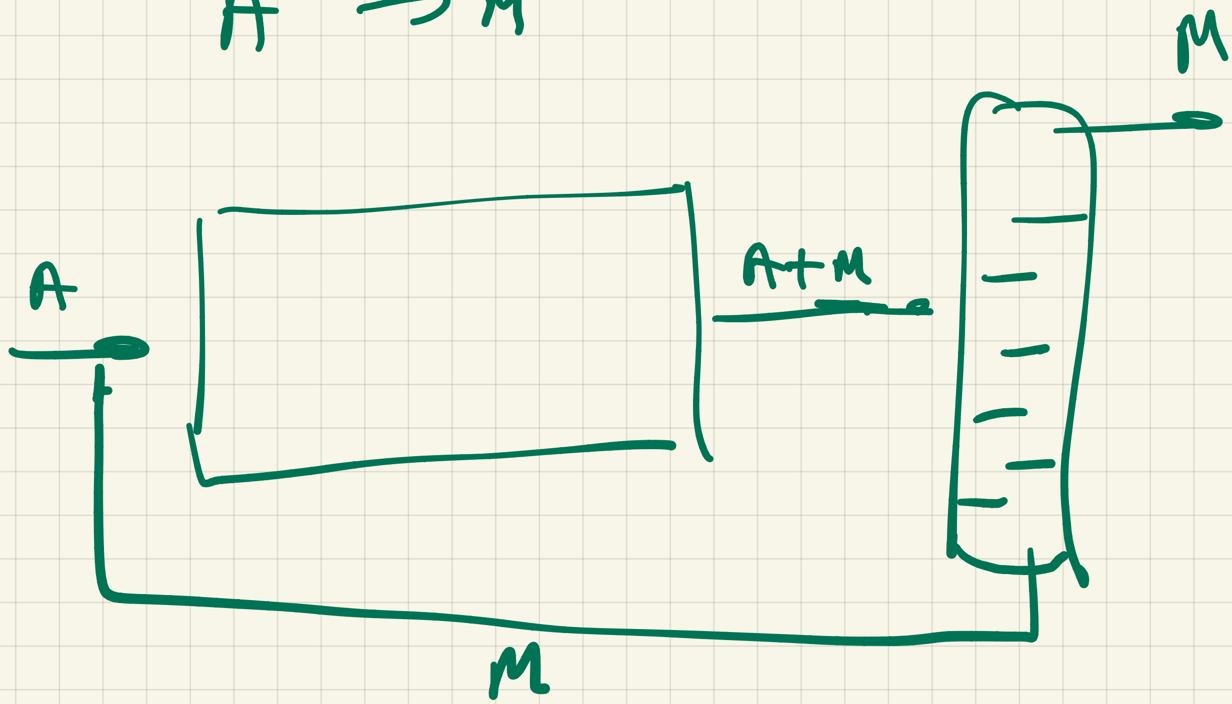
$$\frac{C_{Ac}}{C_A^0} = \frac{1}{1 + k\frac{V}{Rq}}$$

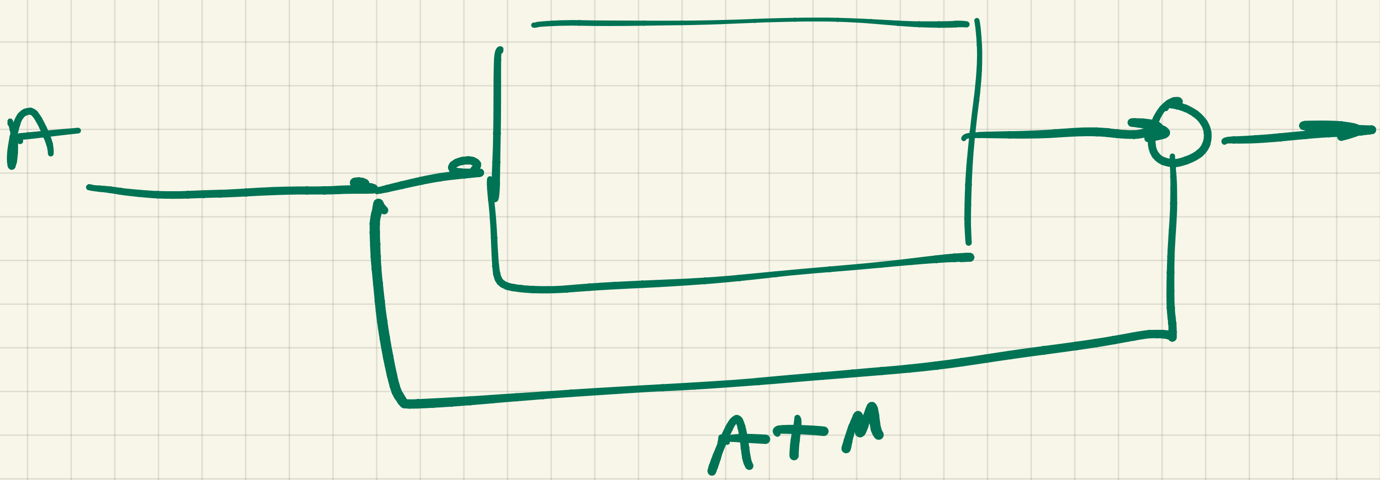
τ INSIDE REACTOR

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

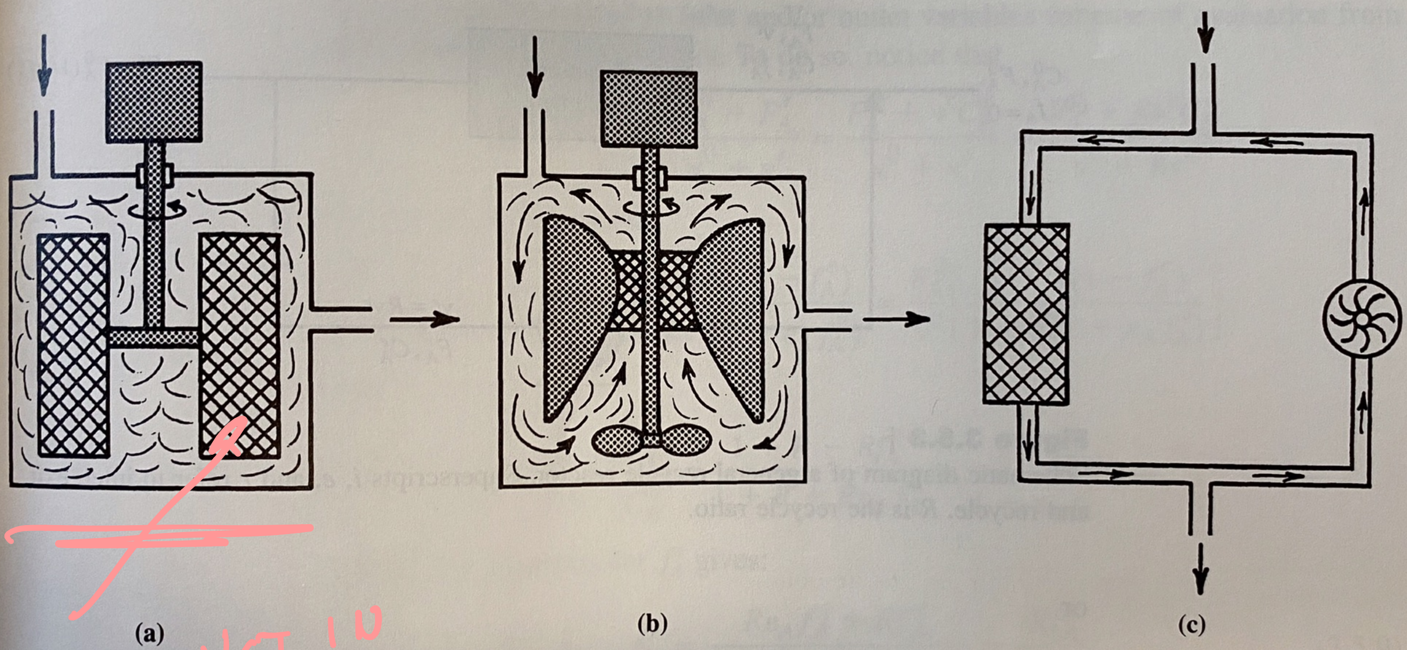
MORE COMMON USE OF RECYCLE:

$A \rightarrow M$





M IS A DILUENT



CATALYST IN "BASKET" THAT IS STIRRED FOR GOOD MASS TRANSFER

Figure 3.5.2 | Stirred contained solids reactors. [Reproduced from V. W. Weekman, Jr., *AIChE J.*, **20** (1974) p. 835, with permission of the American Institute of Chemical Engineers.] **(a)** Carberry reactor, **(b)** Berty reactor (internal recycle reactor), **(c)** external recycle reactor.

IT IS CONVENIENT FOR THE CATALYST TO BE A SOLID

→ EASY SEPARATION FROM PRODUCTS

WOULD RATHER NOT CRUSH UP CATALYST IN EXPERIMENT OR PROCESS

CAN'T STIR LARGE PARTICLES

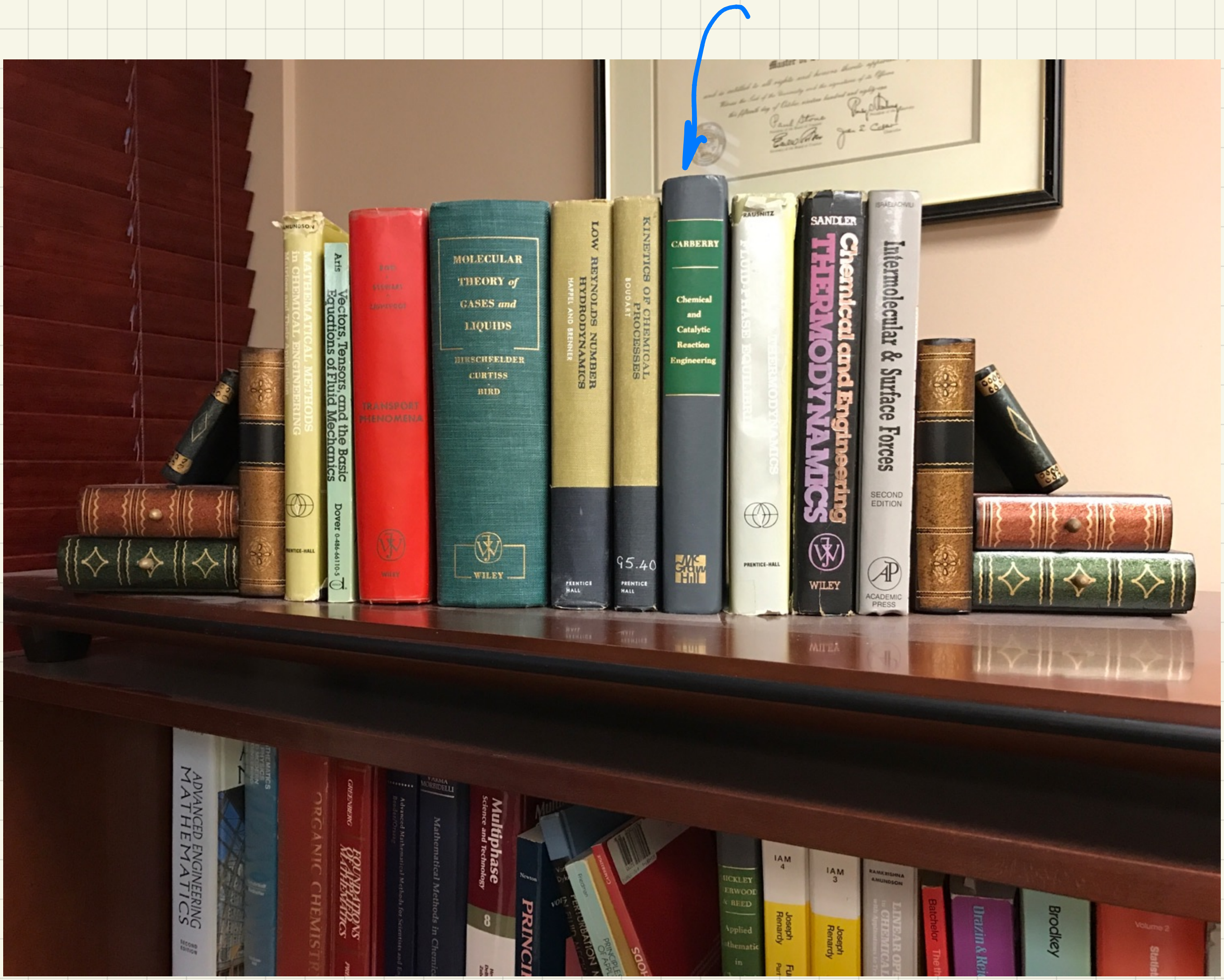
JAMES J. CARBERRY

PROFESSOR AT NOTRE DAME FROM 1963 — 2000

BESIDES PROFESSIONAL ACCOMPLISHMENTS

- FOA (FRIEND OF ARA PARSEGHIAN)
- OPERA AFICIONADO
- INTERHALL FOOTBALL COACH

  ... "GIPP" INCIDENT ...
- TAUGHT CHEG 445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