prelim. review

REACTOR DESIGN

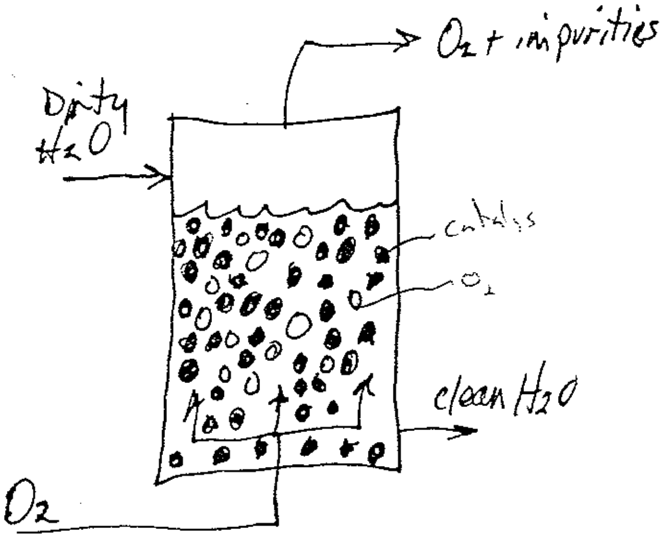
- some basic classifications

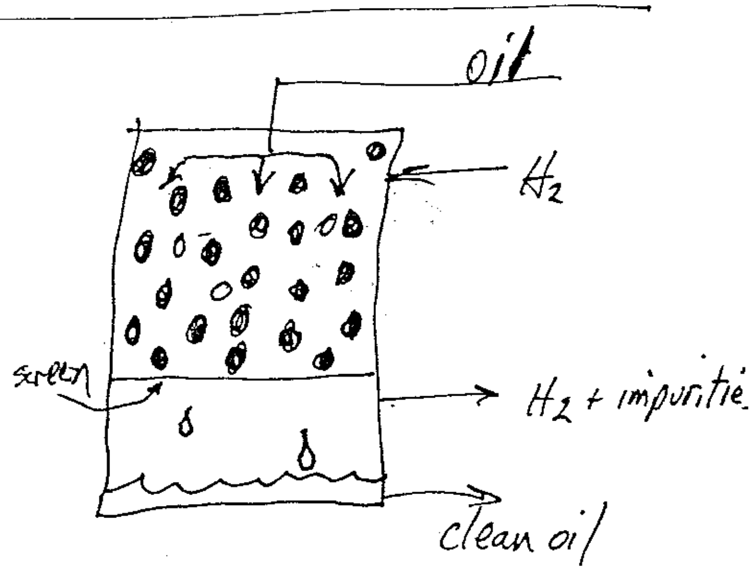
HOMOGENEOUS - 1 phase

- Batch
- Stirred Tank (CSTR, STR) Uniform properties throughout
- Tubular (PFR) complete transverse mixing

HETEROGENEOUS - multiphase

- Fixed Bed - 2 phase *
- Slurry / trickle Bed - 3 phase **
- Fluidized Bed - small catalyst particles *





* - Fixed Bed
or
(Fluidized Bed)
└ raise O_2 velocity to mix catalyst pellets

** - Trickle Bed

REACTOR DESIGN

- basic design procedure

Step I
- bench top analysis of $k(C)^n$, D_e, k
- formulate conservation equations
- characterize mass/heat transfer
- characterize reaction rate
- solve resulting equations

Step II
- pilot plant runs
- measure non idealities (temp. dist, RTD)
- use actual catalyst
- test construction materials

Step III
- full scale production
- optimization operating conditions / feed ratios

REACTOR DESIGN

– ideal design models

CSTR

$$r_i = \frac{dC_i}{dt}$$

– constant volume
– r_i is negative for i = reactan

$$-r_A = C_{A0} \frac{dX_A}{dt}$$

– constant volume
– A is reactant

recycle

$$r_i = \left(\frac{V_R + V_F}{V_R}\right)\frac{dC_i}{dt}$$

– constant volume

PFR

$$r_i = \frac{d(QC_i)}{dV}$$

– non constant volume

$$\text{space velocity} = \frac{V_{Reactor}}{F_A} = \int_{X_F}^{X} \frac{dX_A}{-r_A}$$

– non constant volume
– A is reactant

CSTR's in Series

1st order

$$X = 1 - \frac{1}{\left(1 + k_1 \frac{\bar{\theta}_t}{n}\right)^n}$$

$\bar{\theta}_t \equiv$ total residence time for system

$n \equiv$ # of reactors in series

REACTOR DESIGN

– example problem

Find conversion to Allyl Chloride as a function of length of reactor.

Given

$F_f = 0.85 \frac{\text{lbmol}}{\text{hr}}$ < 4 moles C_3H_6 propylene, 1 mol Cl_2

cooled reactor – 392 °F $h = 5 \frac{\text{Btu}}{\text{hr ft}^2 \text{°F}}$

2 inch id tube , $P = 29.4$ psia

① $Cl_2 + C_3H_6 \xrightarrow{k_1} CH_2{=}CH{-}CH_2Cl + HCl$

Propylene   Allyl Chloride

② $Cl_2 + C_3H_6 \xrightarrow{k_2} CH_2Cl{-}CHCl{-}CH_3$ *

Dichloropropane

$\Delta H_1 = -48{,}000 \text{ Btu/lbmol}$, $\Delta H_2 = -79{,}200 \text{ Btu/lbmol}$

$r_1 = 206{,}000\, e^{-27{,}200/RT} P_{C_3H_6} P_{Cl_2}$ want high T?

$r_2 = 11.7\, e^{-6860/RT} P_{C_3H_6} P_{Cl_2}$

– example problem (cont)

write rate equations in terms of conversion

$$r_1 = 824{,}000\ e^{-13{,}700/T}\ \frac{[0.8-X_1-X_2][0.2-X_1-X_2]}{(1-X_2)^2}$$

$$r_2 = 46.8\ e^{-3460/T}\ \frac{[0.8-X_1-X_2][0.2-X_1-X_2]}{(1-X_2)^2}$$

$$\frac{dT}{dz} = \frac{\pi d\,h\,(T_S-T) - \left(r_1\,\Delta H_{r_1} + r_2\,\Delta H_{r_2}\right)\frac{\pi d^2}{4}}{(F_t\,C_p)}$$

Assume $F_t C_p$ is constant $\cong 18.5$ Btu/hr °F

T, X_1, X_2 are unknowns, z is indep. variable

Numerical Solution – Euler Method (or Runge Kutta)

$$F_t C_p\,\Delta T = \left[\pi d h (T_S - T)_{Ave} - r_1 \Delta H_{r_1} + r_2 \Delta H_{r_2}\ \frac{\pi d^2}{4}\right] \Delta Z$$

$$\Delta X_1 = \bar{r}_1\ \frac{\pi d^2}{4F_t}(\Delta Z)$$

$$\Delta X_2 = \bar{r}_2\ \frac{\pi d^2}{4F_t}(\Delta Z)$$

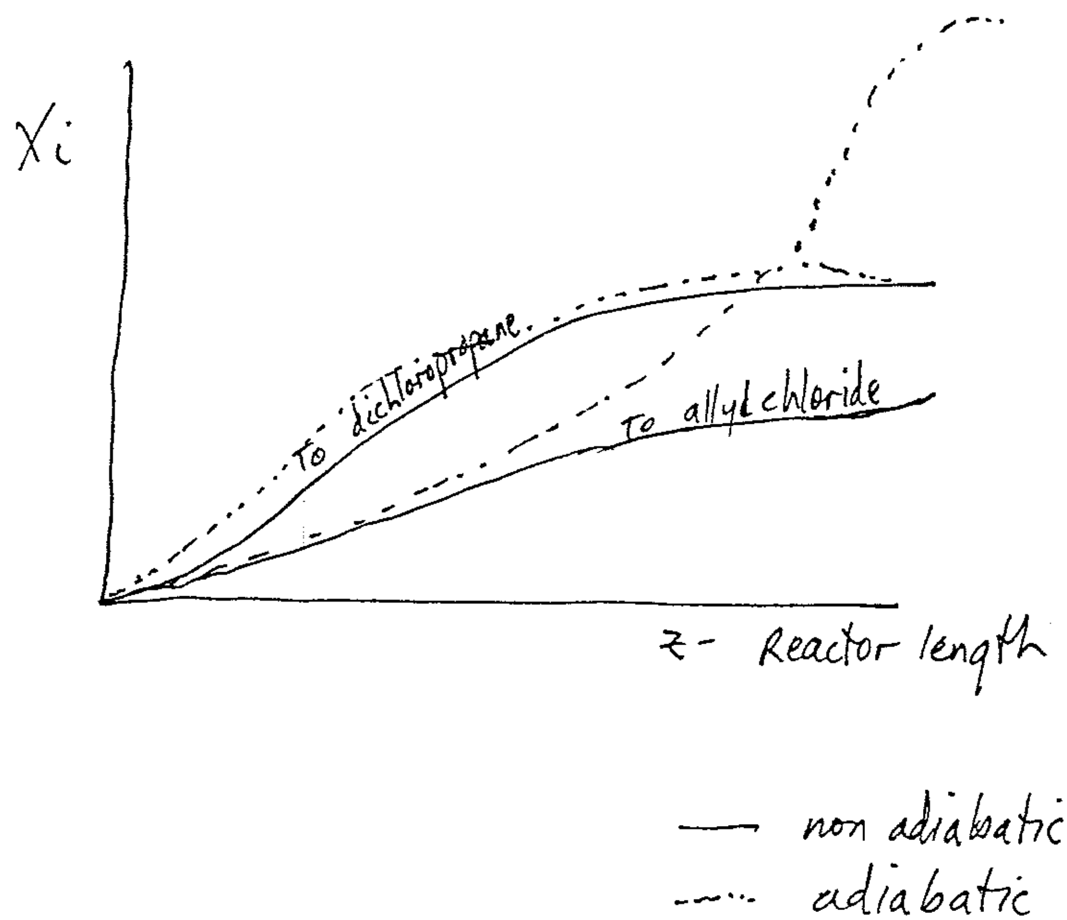
Procedure

1. $T_1 = 392\,°F$, $X_1 = X_2 = 0$ – calculate initial r_1 and r_2
2. choose ΔZ, calculate $\Delta X_1, \Delta X_2$

iterate
3. calculate ΔT by trial and error
4. recalculate r_1 and r_2 at new temperature
5. calculate new $\Delta X_1, \Delta X_2$

— example problem (cont)

Results

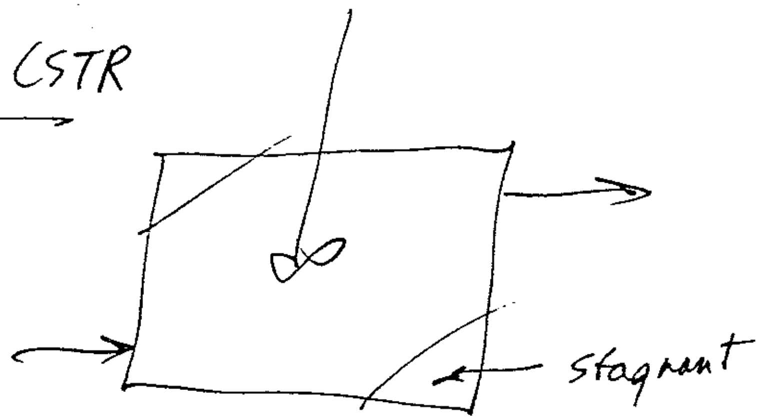


Better conversion by rxn 1 to allyl chloride in adiabatic operation due to the higher activation energy of rxn 1.

REACTOR DESIGN

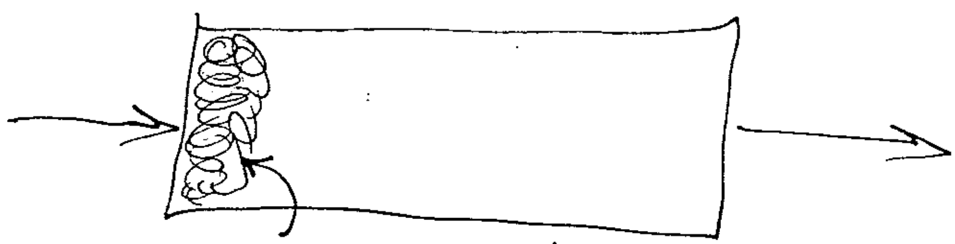
- nonidealities

Batch or CSTR



result: less effective volume
lower conversion rate

Tubular or PFR



Turbulance - longitudinal or axial mixing
"Micromixing"

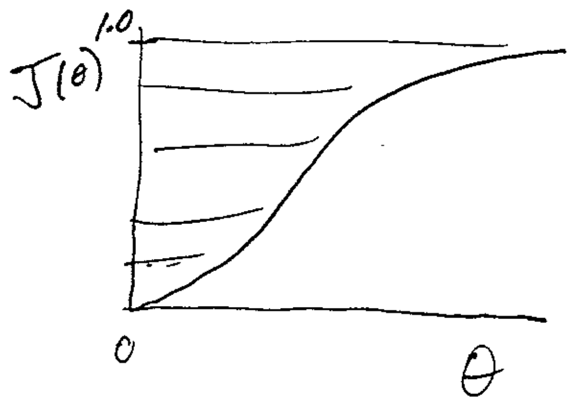
channelling or streamlining - incomplete radial mixing
"Segregated Flow"

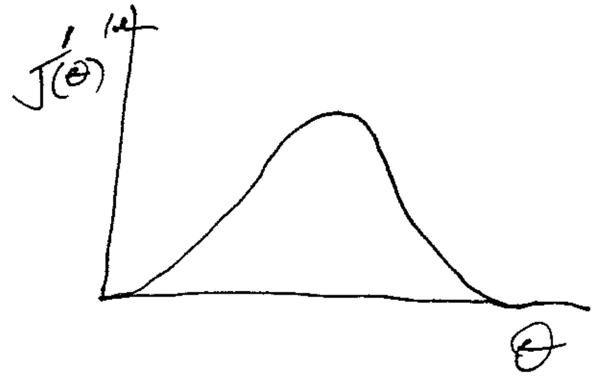
result: lower conversion poor selectivity

REACTOR DESIGN

— Pilot plant study : RTD in PFR (non ideal)

Residence Time Distribution - RTD

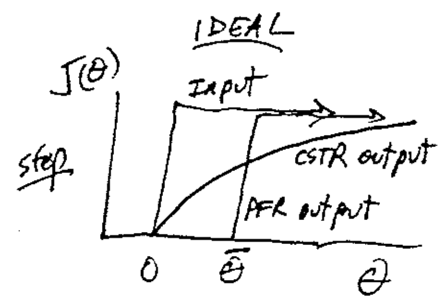


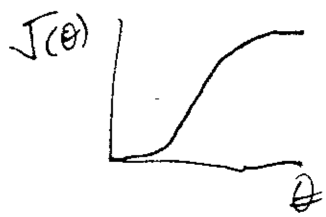


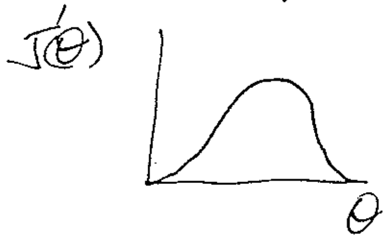
$J(\theta) \equiv$ fraction of effluent stream with $RT < \theta$

Step Change to Input

$$J(\theta) = \left(\frac{C}{C_0}\right)_{step}$$

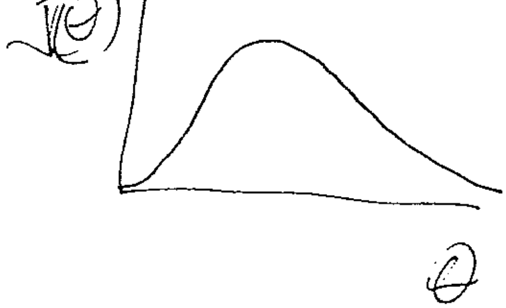


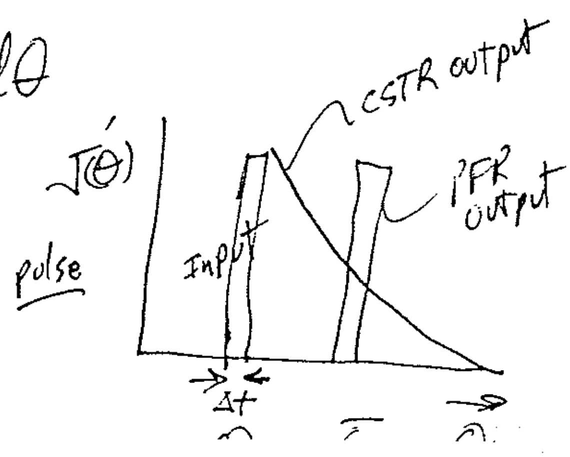




Pulse Input

$$J(\theta) = \frac{\int_0^\theta C_{pulse}\, d\theta}{\int_0^\infty C_{pulse}\, d\theta}$$





REACTOR DESIGN

- RTD (cont.)

How to use measured RTD's to calculate conversion vs. θ (residence time)

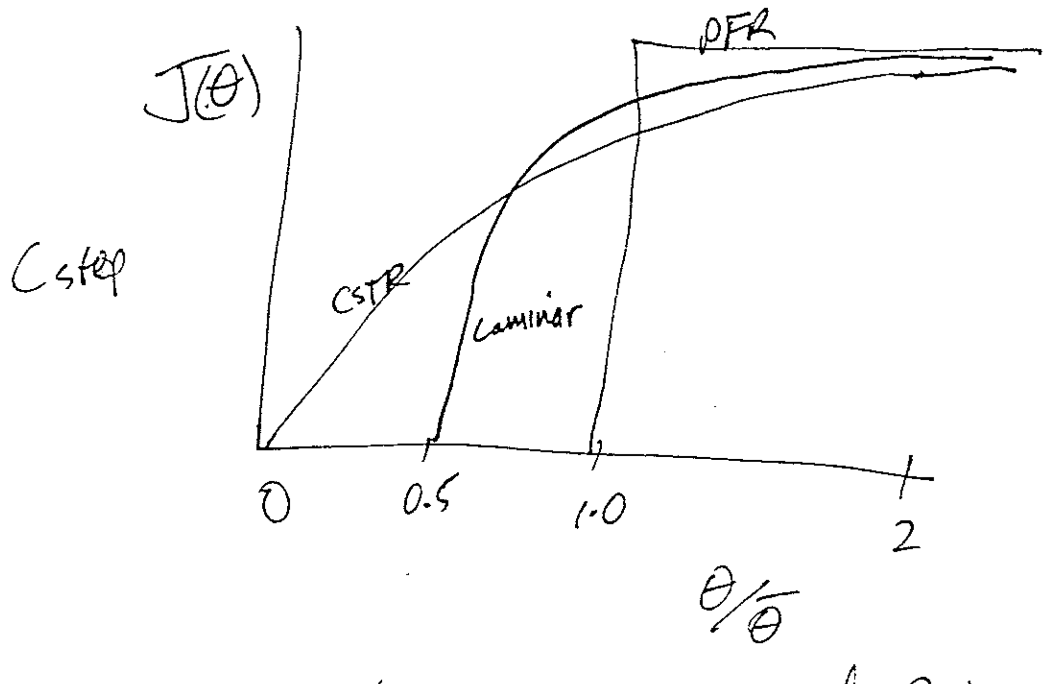
① Assume segregated flow and no micromixing

ex/ Laminar $\quad v(r) = \frac{2Q}{\pi R^2}\left[1-\left(\frac{r}{R}\right)^2\right]$

$$J(\theta) = 1 - \frac{1}{4}\left(\frac{\theta}{\bar{\theta}}\right)^{-2}$$

$$J'(\theta) = \frac{1}{2}\frac{\bar{\theta}^2}{\theta^3}$$

$$\bar{X} = \int_0^\infty X(\theta)\, J'(\theta)\, d\theta$$



— see how your measured RTD fits model —

REACTOR DESIGN

- RTD (cont)

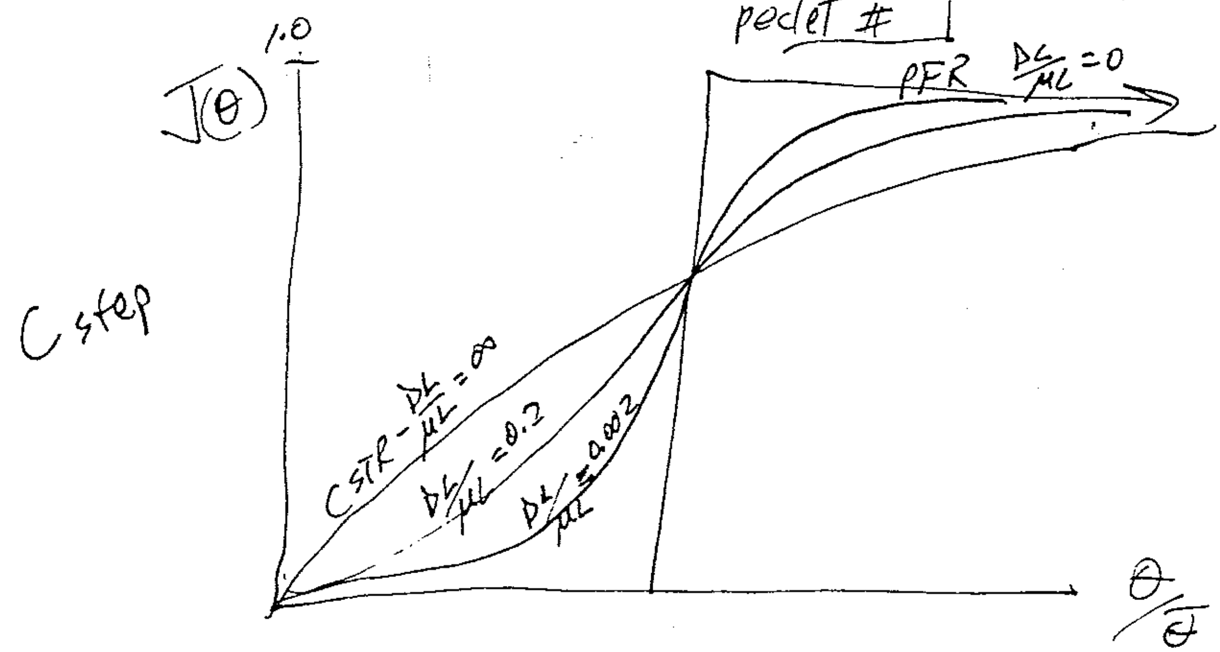
② Axial Dispersion Model

assume axial dispersion, calculate D_e (determine)

$$D_L \frac{\delta^2 C}{\delta z^2} - \mu \frac{\delta C}{\delta z} = \frac{\delta C}{\delta \theta}$$

$$J(\theta) = \frac{1}{2}\left[1 - \operatorname{erf}\left(\frac{1}{2}\sqrt{\frac{\mu L}{D_L}}\left(\frac{1-\theta/\bar{\theta}}{\sqrt{\theta/\bar{\theta}}}\right)\right)\right]$$

peclet #



$$X = 1 - \frac{4\beta}{(1+\beta)^2 e^{-\frac{1}{2}\left(\frac{\mu L}{D_L}\right)(1-\beta)} - (1-\beta)^2 e^{-\frac{1}{2}\left(\frac{\mu L}{D_L}\right)(1-\beta)}}$$

$$\beta = \left(1 + 4k_1\bar{\theta}\,\frac{D_L}{\mu L}\right)^{1/2}$$

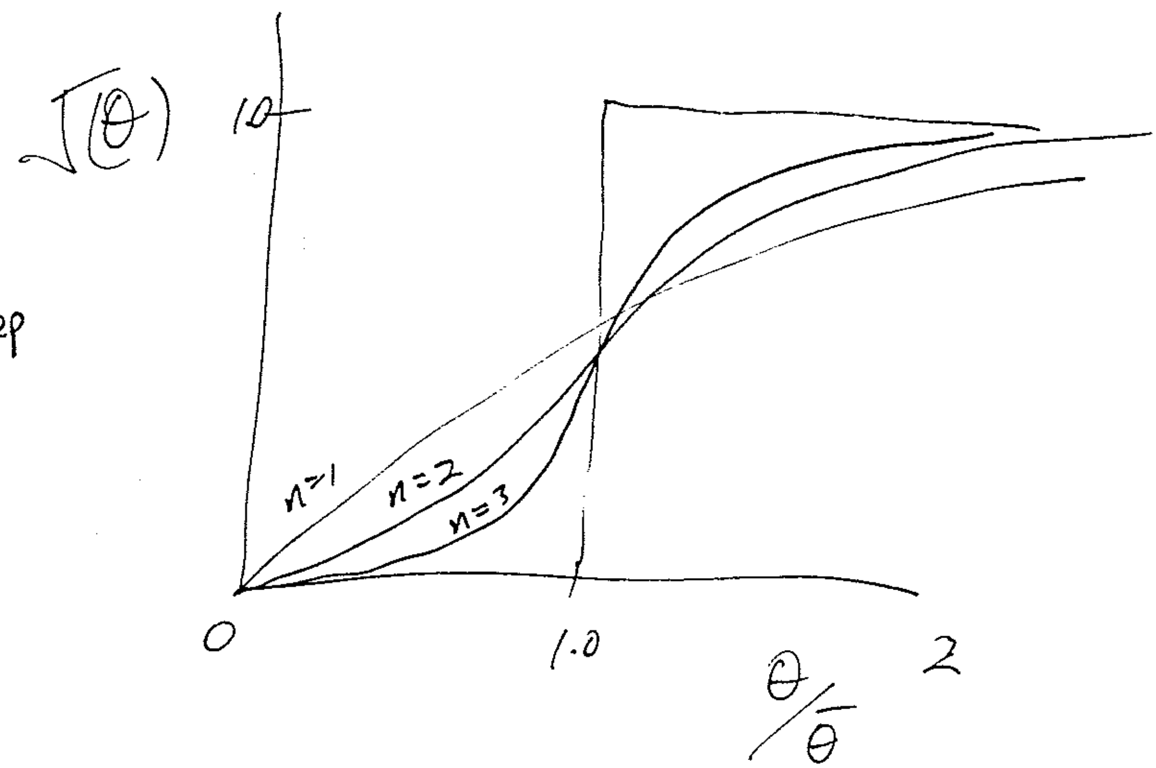
1st order

REACTOR DESIGN

- RTD (cont.)

(3) CSTR IN SERIES MODEL - calculate n (determine)

$$J(\theta) = 1 - e^{-\frac{n\theta}{\bar{\theta}_t}}\left[1 + \frac{n\theta}{\bar{\theta}_t} + \frac{1}{2!}\left(\frac{n\theta}{\bar{\theta}_t}\right)^n + \cdots (n-1\right.$$



for 1st order

$$X = 1 - \frac{1}{\left(1 + k\frac{\bar{\theta}_t}{n}\right)^2}$$

REACTOR DESIGN

- pick a reactor

What to consider

- cost (equipment, labor)
- Operating conditions (P, T)
- Heat Transfer requirements
- Mass Transfer requirements
- selectivity

Batch - small scale, expensive materials

Stirred Tank - good for slow reaction rates, liquids, lower equipment costs

Tubular Flow - higher conversions, gas phase, better heat transfer, lower labor costs

Fixed Bed, slurry/Trickle Bed - multiphase

Fluidized Bed - good mass transfer (order of magnitude better than fixed), good heat transfer, easy catalyst regen → large equipment

REACTOR DESIGN

$r = KC$

$r = k$ ~~...~~

driving force (rate) in CSTR is
in PFR is ~~...~~
$r = KC_{(x)}$

- questions

① PFR's typically give higher conversion as a function of residence time. Why?

② Which type of reactor is best for promotion of one rxn over another (selectivity)

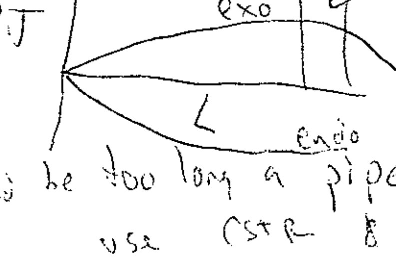
better temp control — PFR or CSTR

③ What kind of reactor is used for

- Petroleum cracking — homogeneous flow (fluidized)
- Ammonia synthesis — gas PFR
- Naphthalene → phthalic anhydride — flow catalyst
- Light hydrocarbon cracking — homogeneous flow tubular rxtr

④ Does conversion depend on temperature in a CSTR? Yes ⟷ size

⑤ What does the temperature distribution in a PFR look like?



hot spot can kill catalyst @ this spot

would be too long a pipe
use CSTR & "staged"

PFR → CSTR