

Design Aspects - based on Shinnar's case study

Processing

- Batch - semi batch
- Solids in plug flow
- Solids in backmix flow

Analysis very much simplified if fluid assumed uniform throughout the reactor i.e. excess of fluid & recycling!

Residence time distribution of solids in reactor needed.

For particles of uniform size the derived equations apply directly

Particles of different sizes PFR of solids, uniform gas comp. (even gas)

sizes  $R_i$   $R_{min} \leq R_i \leq R_{max}$   
say  $R_i$  identified directly by screening

Feed in the reactor

$$F = \sum_{R_i=R_{min}}^{R_i=R_{max}} F(R_i) \quad (1)$$

Residence time in reactor for all solids  $\bar{t}_p = \frac{V_d t_c}{F}$

F - defined as volumetric feed rate of solids, when density does not change appreciably it is equivalent to the mass feed rate

Find  $X_B(R_i)$  for any particle size from the derived equations, using the knowledge of the rate controlling step.

The mean conversion is then given by.

$$\left( \begin{array}{l} \text{mean value} \\ \text{of fraction of} \\ \text{unreacted B} \end{array} \right) = \sum \left( \begin{array}{l} \text{fraction of} \\ \text{reactant unreacted} \\ \text{in solids of size } R_i \end{array} \right) \left( \begin{array}{l} \text{fraction of} \\ \text{feed of} \\ \text{size } R_i \end{array} \right)$$

$$1 - \bar{x}_B = \sum_{R_{min}}^{R_{max}} [1 - x_B(R_i)] \frac{F(R_i)}{F} \quad 0 \leq x_B \leq 1$$

OR in equivalent form

$$1 - \bar{x}_B = \sum_{R(t_0=\tau)}^{R_{max}} [1 - x_B(R_i)] \frac{F(R_i)}{F}$$

This model might be applied to moving beds  
example lecture 9 p 22 ; Problem P2A

Particles of single size backmix flow of solids, uniform gas  
 Applicable to fluidized beds without carryover

The length of stay is now different for the particles : some come out early some late

$$\left( \begin{array}{l} \text{mean value} \\ \text{for fraction} \\ \text{of B} \\ \text{unreacted} \end{array} \right) = \sum_{\text{all ages}} \left( \begin{array}{l} \text{fraction of B} \\ \text{unreacted for} \\ \text{particles staying} \\ \text{in the reactor} \\ \text{for time between } t \text{ and } t+dt \end{array} \right) \left( \begin{array}{l} \text{fraction of} \\ \text{exit stream} \\ \text{which stayed} \\ \text{in reactor} \\ \text{between } t \text{ and } t+dt \end{array} \right)$$

$$1 - \bar{x}_B = \int_0^{\infty} [1 - x_B(t)] E(t) dt = \int_0^{\tau} [1 - x_B(t)] E(t) dt$$

find from derived equations using

the knowledge of the controlling step.

$$E(t) = \frac{1}{\tau} e^{-t/\tau}$$

$$\frac{\partial P}{\partial t} \quad 1 - \bar{x}_B = \int_0^{\tau} [1 - x_B(t)] E(t) dt$$

Mixture of particles, CSTR of solids, uniform gas

Applicable to fluidized beds, (solid discharge)

Since we have steady state: no change in particle size and the exit stream is representative of bed conditions. The size distributions in the bed, feed & exit stream must be alike.

$$\frac{F(R_i)}{F} = \frac{W(R_i)}{W} \text{ in reactor} = \frac{F_i(R_i)}{F_i}$$

The mean residence time for any size is equal to the mean residence time of solid.

$$\bar{t} = \bar{t}(R_i) = \frac{W}{F}$$

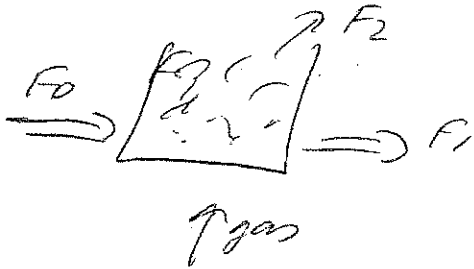
Then mean conversion for size  $R_i$

$$1 - \bar{x}_B(R_i) = \int_0^{\infty} [1 - x_B(R_i, t)] E(t) dt$$

The mean conversion for all solids:

$$1 - \bar{x}_B = \sum_{R_{min}}^{R_{max}} [1 - \bar{x}_B(R_i)] \frac{F(R_i)}{F}$$

Mixed gas flow & solids flow  
reactor with electric heat



$$F_1 = \sum F_i(R_i)$$

$$F_0(R_i) = F_1(R_i) + F_2(R_i)$$

$$F_2(R_i) = \kappa(R_i) W(R_i)$$

$$\frac{F_1(R_i)}{W(R_i)} \equiv \frac{F_1}{W}$$

same to all  
reactor  
amount of well  
mixedness

$$F_0(R_i) = F_1(R_i) + \kappa(R_i) \frac{W}{F_1} F_1(R_i)$$

$$F_0(R_i) = F_1(R_i) \left[ 1 + \kappa(R_i) \frac{W}{F_1} \right]$$

$$(*) \quad F_0 = \sum F_0(R_i) = \sum \frac{F_0(R_i)}{1 + \kappa(R_i) \frac{W}{F_1}}$$

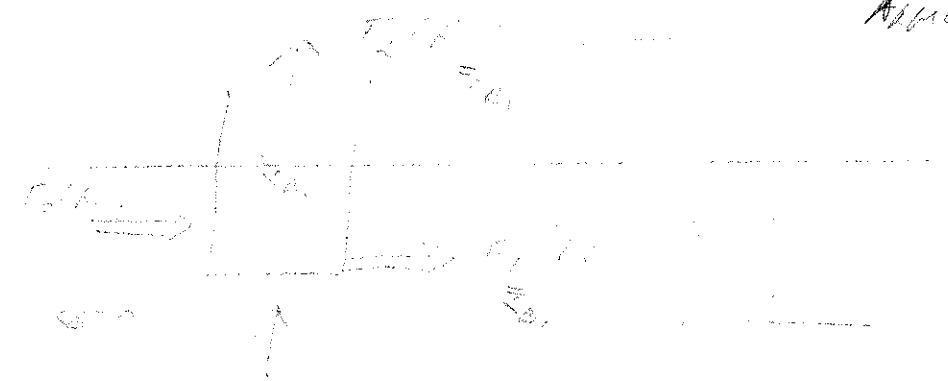
$$\bar{E}(R_i) = \frac{W(R_i)}{F_1(R_i) + F_2(R_i)} = \frac{1}{\frac{F_1}{W} + \kappa(R_i)}$$

$$F_2(R_i) = \kappa(R_i) \frac{F_1(R_i)}{F_1} W = \kappa(R_i) W(R_i)$$

$$1 - \bar{X}_B = \int_0^E (1 - X_B(R_i)) \bar{E}(R_i) dR_i$$

$$1 - \bar{X}_B = \sum (1 - X_B(R_i)) \frac{F_0(R_i)}{F}$$

Approximate 1/2 cent



All solids have exponential RTD but their mean residence time depends on size

- (1)  $F_0 = \sum F_i$
- (2) Table of  $F_i$  vs  $R_i$
- (3)  $\int \frac{F_i(t)}{F_0} dt = 1$   $\Rightarrow$  are distributions in the reactor

$$(4) \bar{t}(R_i) = \frac{\int_0^\infty t F_i(t) dt}{F_i} = \frac{w(R_i)}{F_i} = \frac{1}{\frac{F_i}{w} + \kappa(R_i)}$$

$$(5) \bar{t}(R_i) = \int_0^\infty t F_i(t) dt = \frac{w(R_i)}{F_i} \Rightarrow \bar{t}(R_i) = \frac{1}{\frac{F_i}{w} + \kappa(R_i)}$$

as  $R_i \downarrow \kappa(R_i) \uparrow$

$$A(R_i) = \frac{F_0(t)}{w(R_i)} \quad \bar{t}(R_i) = \frac{1}{\frac{F_i}{w} + \kappa(R_i)} = \frac{w(R_i)}{F_i}$$

$$(*) \quad \bar{t} = \sum_{i=1}^n F_i(R_i) = \sum_{i=1}^n \frac{F_i}{w} w(R_i) = \sum_{i=1}^n \frac{F_i}{w} \frac{F_0(R_i)}{\frac{F_i}{w} + \kappa(R_i)} = \sum_{i=1}^n \frac{F_0(R_i)}{1 + \frac{w}{F_i} \kappa(R_i)}$$

$F_i(R_i) = \frac{F_0(R_i)}{1 + \frac{w}{F_i} \kappa(R_i)}$   
(over)

Given:  $F_0(R_i)$ ,  $W$ ,  $x(R_i)$   
 solve for  $F_1$  by trial and error  
 from  $(x)$   
 i.e. guess  $F_1$ , get  $F_1(R_i)$  and sum  
 to get  $F_1$ .

Then

$$\left( \begin{array}{l} \text{fraction of} \\ \text{all solids unconverted} \end{array} \right) = \sum_{\text{all } n \text{ res}} \left( \begin{array}{l} \text{fraction} \\ \text{of } n \text{ res} \\ \text{unconverted} \end{array} \right) \left( \begin{array}{l} \text{fraction of} \\ \text{that } n \text{ res} \\ \text{is the feed} \end{array} \right)$$

$$1 - \bar{x}_B = \sum_{R_i=R_{min}}^{R_{max}} [1 - \bar{x}_B(R_i)] \frac{F_0(R_i)}{F_0}$$

This means that conversion is defined on total solids:

$$\bar{x}_B = \frac{F_{B0} - (F_{1B} + F_{2B})}{F_{B0}}$$

This can be written as:

$$1 - \bar{x}_B = \frac{F_1(1 - \bar{x}_{Bov}) + F_2(1 - \bar{x}_{Bel})}{F_0}$$

where

$$1 - \bar{x}_{Bov} = \sum_{R_i=R_{min}}^{R_{max}} [1 - \bar{x}_B(R_i)] \frac{F_1(R_i)}{F_1}$$

$$1 - \bar{x}_{Bel} = \sum_{R_i=R_{min}}^{R_{max}} [1 - \bar{x}_B(R_i)] \frac{F_2(R_i)}{F_2}$$

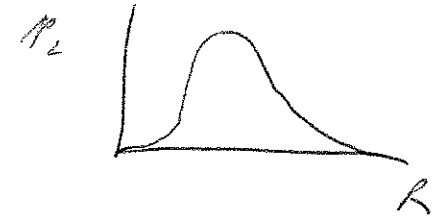
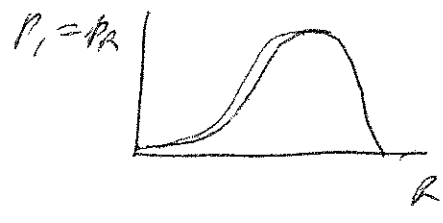
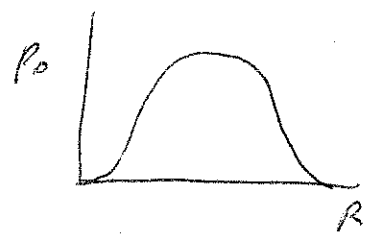
$$\bar{x}_{Bov} = \frac{F_1 - F_{1B}}{F_1}$$

$$F_{1B} = F_1(1 - \bar{x}_{Bov})$$

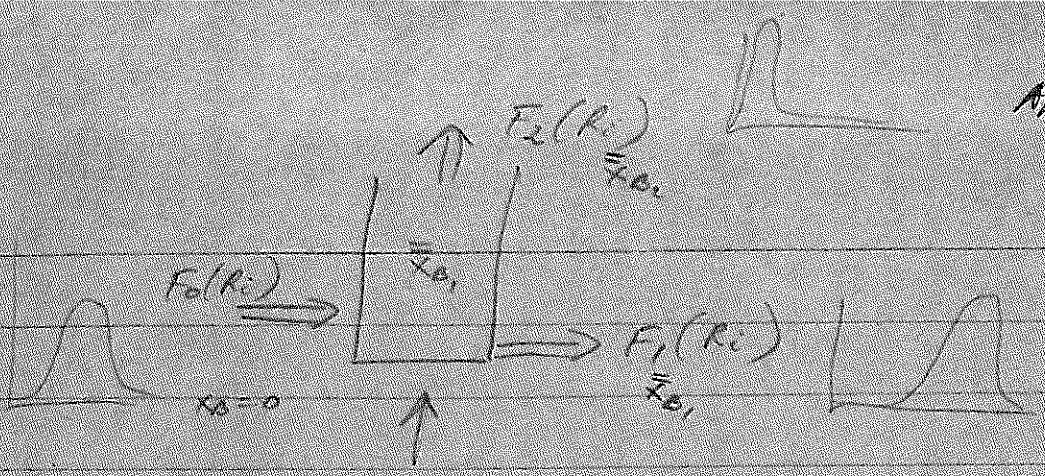
Some problem can be approached from the point of view of continuous size distribution here

$$P_0(R) \neq P_1(R) = P_R(R) \Rightarrow P_2(R)$$

$$F_1(R) = \int F_1 P_1(R) dR$$
$$W_1(R) = \int W_1 P_R(R) dR$$



Approximate 1st cut



All solids have exponential RTD but temp more variable  
fine deposits on size

(1)  $F_0 = F_1 + F_2$

(2)  $F_0(R_i) = F_1(R_i) + F_2(R_i)$

perfect mixing assumption requires

(3)  $\left| \frac{F_1(R_i)}{F_1} = \frac{W(R_i)}{W} \right| \Rightarrow$  one distribution will be small

Different  $\bar{E}(R_i)$  for various  $R_i$

(4)  $\bar{E}(R_i) = \frac{W(R_i)}{F_0(R_i)} = \frac{W(R_i)}{F_1(R_i) + F_2(R_i)} = \frac{1}{\frac{F_1}{W} + \frac{F_2(R_i)}{W(R_i)}}$

(5)  $1 - \bar{X}_B(R_i) = \int_0^{R_i} [1 - X_B(R_i)] \frac{e^{-t/\bar{E}(R_i)}}{\bar{E}(R_i)} dt$   $\bar{E}(R_i) = \frac{1}{\frac{F_1}{W} + \frac{F_2(R_i)}{W(R_i)}}$

$1 - \bar{X}_B = \sum_{R_i} [1 - \bar{X}_B(R_i)] \frac{F_0(R_i)}{F_0}$   $\text{as } R_i \downarrow \Rightarrow \frac{F_2(R_i)}{W(R_i)} \downarrow$

$\frac{d(\text{no. of tracer particles})}{dt} = \kappa (\text{number of tracer particles})$

$\kappa \sim \frac{(\text{gas velocity})^2}{(\text{bed height})(\text{particle size})^{2.65}}$

$\kappa(R_i) = \frac{F_2(R_i)}{W(R_i)}$   $\bar{E}(R_i) = \frac{1}{\frac{F_1}{W} + \kappa(R_i)} = \frac{W(R_i)}{F_0(R_i)}$

(\*)  $F_1 = \sum_{R_i} F_1(R_i) = \sum_{R_i} \frac{F_1}{W} W(R_i) = \sum_{R_i} \frac{F_1}{W} \frac{F_0(R_i)}{\frac{F_1}{W} + \kappa(R_i)} = \sum_{R_i} \frac{F_0(R_i)}{1 + \frac{W}{F_1} \kappa(R_i)}$

$F_1 = \sum_{R_i} \frac{F_0(R_i)}{1 + \frac{W}{F_1} \kappa(R_i)}$   $F_1(R_i) = \frac{F_0(R_i)}{1 + \frac{W}{F_1} \kappa(R_i)}$   
That's it (over)



12-25

Elasticity experiment

$$\frac{dP(R_i)}{dt} = \kappa P(R_i)$$

$$-\ln \frac{P(R_i)_{t=t}}{P(R_i)_{t=0}} = \kappa(R_i) t$$

$$\kappa(70) = \frac{1}{2} \ln \frac{450}{36} = 1.263$$

$$\kappa(98) = \frac{1}{2} \ln \frac{450}{159} = 0.52$$

$$\kappa(116) = \frac{1}{2} \ln \frac{450}{302} = 0.196$$

$$\kappa(R) = 1.3 \times 10^{-4} (\text{yr}^{-2.6} \text{ mm}^{-1}) R^{-2.6}$$

