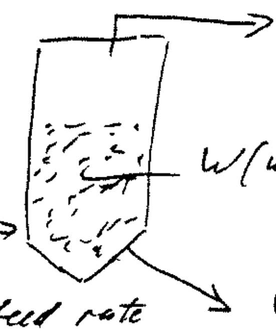
Modeling of Noncatalytic Fluidized Bed Reactors

This is a very broad area and we will restrict our attention to the situation when we have growing or shrinking particles <u>only</u>.



$\dot{w}_2\left(\frac{kg}{h}\right)$ – mass flow rate of the carryover stream

$W(kg)$ – mass of fluidized bed

$\dot{w}_0\left(\frac{kg}{h}\right)$ – total feed rate of solids (mass feed rate)

$\dot{w}_1\left(\frac{kg}{h}\right)$ – mass flow rate of the underflow stream

$$\dot{w}_1 + \dot{w}_2 > \dot{w}_0 \quad \rightarrow \text{particle growth}$$

$$\dot{w}_1 + \dot{w}_2 < \dot{w}_0 \quad \rightarrow \text{particle shrinkage}$$

The general differential equation describing this system is obtained by a population balance:

$$0 = \underbrace{\dot{w}_0 p_0(R)}_{\substack{\text{input rate}\\ \text{of particles of}\\ \text{size } R \text{ to}\\ R+dR}} \underbrace{- \dot{w}_1 p_1(R)}_{\substack{\text{output rate}\\ \text{by underflow}\\ \text{of particles of}\\ \text{size } R \text{ to } R+dR}} \underbrace{- W \mathcal{K}(R) p_1(R)}_{\substack{\text{output rate by}\\ \text{elutriation of}\\ \text{particles of size}\\ R \text{ to } R+dR}} \underbrace{- W \frac{d[\mathcal{R}(R) p_1(R)]}{dR}}_{\substack{\text{net rate of solids}\\ \text{growing into this}\\ \text{size interval and}\\ \text{out of it}}} + \underbrace{\frac{3W}{R} p_1(R) \mathcal{R}(R}_{\substack{\text{solid generat.}\\ \text{due to growth}\\ \text{within the}\\ \text{interval}\\ \text{assuming}\\ \text{spherical}\\ \text{particles}}}$$

$p(R)\,dR$ – ~~mass~~ mass fraction of solids in the interval between R & $R+dR$

$p_0(R)$, $p_1(R)$, $p_2(R)$ – probability density functions describing particle size distribution in the feed, bed & underflow and overflow stream, respectively

$R(R)$ — rate of change of particle size: to be found experimentally

$$R(R) = \begin{cases} -k \\ -\frac{k'}{R} \\ -\frac{k''}{R^{1/2}} \end{cases} \quad \text{particle shrinkage}$$

$$R(R) = \begin{cases} k \\ \frac{k'}{R} \\ \frac{k''}{R^{1/2}} \\ k'''R \end{cases} \quad \text{particle growth}$$

⟹ In the above a <u>uniform</u> gas composition is assumed in the bed.

$\mathcal{K}(R)$ (s^{-1}) — elutriation constant for particles of size R

Elutriation refers to selective removal of fines by entrainment from a bed consisting of a mixture of particle sizes.

$$-\frac{1}{A_t}\frac{dW(R)}{dt} = K^* \frac{W(R)}{W}$$

$K^*\left(\frac{g}{cm^2\, s}\right)$ — depends on solid size

Also

$$-\frac{dW(R)}{dt} = \mathcal{K}\, W(R)$$

$$\mathcal{K}^* = \frac{\mathcal{K}\, W}{A_t}$$

$\frac{\mathcal{K}^* d_p}{\mu}\ \frac{g\, d_p}{(u_o - u_t)^2}$ vs $\frac{d_p u_t \rho}{\mu}$ available as a correlation.

~~[illegible]~~ Better to take data on system of interest.

For a <u>single size</u> feed of particles R_o one gets

$$\frac{W}{\dot{w}_o} = \int_{R_o}^{R(t\to\infty)} \frac{R^3}{\mathcal{R}(R)\, R_o^3}\, I(R, R_o)\, dR \qquad (A1) \quad (4)$$

where

$$I(R, R_o) = \exp\left[-\int_{R_o}^{R} \frac{\dot{w}_1/W + \varkappa(R)}{\mathcal{R}(R)}\, dR\right] \qquad \text{(DEF)} \quad (A2)$$

The size distribution in the bed is

$$p_1(R) = \frac{\dot{w}_o}{W\,|\mathcal{R}(R)|}\, \frac{R^3}{R_o^3}\, I(R, R_o) \, . \qquad (A3) \quad (3)$$

Overall balance gives

$$\dot{w}_1 + \dot{w}_2 - \dot{w}_o = \int_{\text{all } R} \frac{3\, W\, p_1(R)\, \mathcal{R}(R)\, dR}{R} \qquad (A4) \quad (2)$$

$$p_2(R) = \frac{W}{\dot{w}_2}\, \varkappa(R)\, p_1(R) \qquad (A5)$$

<u>Example 1:</u> We want to produce 150 kg/h of Si in a fluidized bed

$$SiH_4 = Si + 2H_2$$

seed particles of $R = 100\ \mu m$ are fed into the reactor. We want to produce a surface mean particle size of $\bar{R}_s = 1000\ \mu m$. The growth rate is $100\ \mu m/h$.

Find the size of the reactor W, and seed feed rate $\dot{w}_o$

F_o

First recall that

$p_1(R)\,dR$ — mass fraction of solids in the bed between size R & $R+dR$

The number fraction of solids in the bed between size R & $R+dR$ is:

$$m_1(R)\,dR = \frac{W\,p_1(R)\,dR}{N\,\frac{4}{3}\pi R^3 \rho_s}$$

Mean particle radius based on external surface is defined by:

$$S_{ex} = N\,4\pi \bar{R}_s^2 = N\int_{R_{min}}^{R_{max}} 4\pi R^2 m(R)\,dR = \frac{3W}{\rho_s}\int_{R_{min}}^{R_{max}} \frac{p_1(R)\,dR}{R}$$

$$V = N\,\frac{4}{3}\pi \bar{R}_s^3 = N\int_{R_{min}}^{R_{max}} \frac{4}{3}\pi R^3 m(R)\,dR = \frac{W}{\rho_s}\int_{R_{min}}^{R_{max}} p_1(R)\,dR = \frac{W}{\rho_s}$$

$$\frac{S_{ex}}{V} = \frac{3}{\bar{R}_s} = \frac{\frac{3W}{\rho_s}\int_{R_{min}}^{R_{max}} \frac{p_1(R)\,dR}{R}}{\frac{W}{\rho_s}}$$

$$\boxed{\bar{R}_s = \frac{1}{\int_{R_{min}}^{R_{max}} \frac{p_1(R)\,dR}{R}}}$$

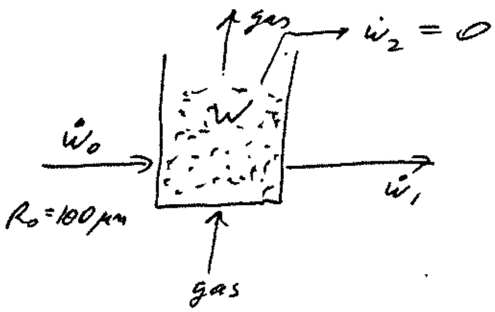
— size of particle whose surface to volume ratio equals that of all solids in the mixture.

Other averages can be defined

$$\bar{R}_w^3 = \frac{1}{\int_{R_{min}}^{R_{max}} \frac{p_1(R)}{R^3}\,dR}$$

$\Longrightarrow$ weight average particle radius i.e. the size of particle whose weight is the mean of all N particles in the mixture

Now let us solve the problem:



no elutriation is assumed

From (A2)

$$I(R, R_0) = e^{\frac{\dot w_1}{kW}(R_0 - R)}$$

since $\mathcal{R}(R) = k = 100\ \mu m/h$

From (A3)

$$p_1(R) = \frac{\dot w_0}{Wk}\,\frac{R^3}{R_0^3}\, e^{\frac{\dot w_1}{kW}(R_0 - R)} \qquad \text{for } R > R_0$$

From (A4)

$$\frac{\dot w_1}{\dot w_0} = 1 + \int_R^{R=\infty} \frac{3}{R_0^3}\, e^{\frac{\dot w_1}{kW}R_0}\; R^2 e^{-\frac{\dot w_1}{kW}R}\, dR$$

$$\frac{\dot w_1}{\dot w_0} = 1 + 3\,\frac{Wk}{\dot w_1 R_0} + 6\left(\frac{Wk}{\dot w_1 R_0}\right)^2 + 6\left(\frac{Wk}{\dot w_1 R_0}\right)^3$$

$$\bar R_s = \frac{1}{\frac{\dot w_0}{Wk R_0^3}\, e^{\frac{\dot w_1}{kW}R_0} \int_{R_0}^{\infty} R^2 e^{-\frac{\dot w_1}{kW}R}\, dR} =$$

$$= \frac{1}{\frac{\dot w_0}{Wk R_0^3}\, e^{\frac{\dot w_1}{kW}R_0}\left[-R^2\frac{kW}{\dot w_1} e^{-\frac{\dot w_1}{kW}R} - 2R\left(\frac{kW}{\dot w_1}\right)^2 e^{-\frac{\dot w_1}{kW}R} - 2\left(\frac{kW}{\dot w_1}\right)^3 e^{-\frac{\dot w_1}{kW}}\right.}$$

$$= \frac{Wk}{\dot w_0\left[\frac{kW}{\dot w_1 R_0} + 2\left(\frac{kW}{\dot w_1 R_0}\right)^2 + 2\left(\frac{kW}{\dot w_1 R_0}\right)^3\right]} = \frac{3Wk}{\dot w_0\left(\frac{\dot w_1}{\dot w_0} - 1\right)}$$

$$\bar R_s = \frac{3\,Wk/\dot w_0}{\frac{\dot w_1}{\dot w_0} - 1}$$

$$\frac{\bar{R}_s}{R_0} = \frac{3\,WK/\dot{w}_0 R_0}{\frac{\dot{w}_1}{\dot{w}_0} - 1}$$

$$\frac{1000}{100} = \frac{3\,W \times 100/\dot{w}_0 \times 100}{\frac{\dot{w}_1}{\dot{w}_0} - 1} = \frac{3\,\frac{W}{\dot{w}_0}}{\frac{\dot{w}_1}{\dot{w}_0} - 1}$$

$$10 = \frac{3\,W}{\dot{w}_1 - \dot{w}_0}$$

$$W = \frac{10}{3}(\dot{w}_1 - \dot{w}_0)$$

Production rate in the fluidized bed $= \dot{w}_1 - \dot{w}_0$

$$150 = \dot{w}_1 - \dot{w}_0$$

$$\boxed{W = \frac{10}{3} \times 150 = 500 \text{ kg}}$$ Required mass of bed

$$\dot{w}_0 = \dot{w}_1 - 150$$

$$\frac{WK}{\dot{w}_1 R_0} = \frac{500 \times 100}{\dot{w}_1 \times 100} = \frac{500}{\dot{w}_1}$$

$$\frac{\dot{w}_1}{\dot{w}_1 - 150} = 1 + 3\left(\frac{500}{\dot{w}_1}\right) + 6\left(\frac{500}{\dot{w}_1}\right)^2 + 6\left(\frac{500}{\dot{w}_1}\right)^3$$

Solve by trial and error

$\dot{w}_1 = 150.5$ kg/h — exit stream

$\dot{w}_0 = 0.5$ kg/h — feed stream of seeds

$W = 500$ kg — bed size

Note that if we wanted to grow particles only up to $\bar{R}_s = 200\,\mu$ $\underbrace{}_{}$ under above conditions we would need a bed of $W =$ 100 kg, the exit stream would be $\dot{w}_1 = 184.5$ kg/h and seeds' feed rate $\dot{w}_0 = 34.5$ kg/h

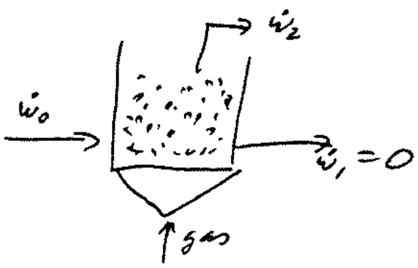
$\boxed{\text{Example 2}}$: We are producing TCS in a fluidized bed

$$Si(s) + H_2(g) + 3SiCl_4(g) = 4SiHCl_3(g)$$

The solids feed consists of a single particle size $R_0 = 200\,\mu m$. These particles under reaction conditions would react completely in 8 h. However the particles shrink to 50 μm and are then entrained out of the bed.

How large a bed do we need to convert 120 kg/h of Si to TCS.

Assume linear shrinkage



$$\mathcal{R}(R) = -k$$

$$\frac{R_0 - R}{k} = t$$

$$k = \frac{R_0 - R}{t} = \frac{200 - 0}{8} = 25\,\mu m/h$$

70 to *

* * This situation is equivalent to plug flow of solids since all solids stay the same time in the reactor i.e

$$\bar{t} = \frac{R_0 - R_{min}}{k} = \frac{200 - 50}{25} = 6\ (h)$$

Last time (Lecture 9) we developed the equation for plug flow of solids and constant shrinkage rate

$$\frac{Wk}{\dot{w}_0 R_0} = \frac{1}{4}\left[1 - \left(\frac{R}{R_0}\right)^4\right] = \frac{1}{4}\left[1 - \left(1 - \frac{k\bar{t}}{R_0}\right)^4\right]$$

$$\frac{25\,W}{200\,\dot{w}_0} = \frac{1}{4}\left[1 - \left(\frac{50}{200}\right)^4\right]$$

$$\frac{W}{\dot{w}_0} = 2\left[1 - \frac{1}{4^4}\right]$$

At the same time since the number of particles in the feed and elutriated stream is the same

$$\frac{\dot{w}_2}{\dot{w}_0} = \left(\frac{R}{R_0}\right)^3 = \left(\frac{50}{200}\right)^3 = \frac{1}{4^3}$$

We want to use 120 kg/h of Si i.e

$$\dot{w}_0 - \dot{w}_2 = 120$$

$$\dot{w}_0\left[1 - \frac{\dot{w}_2}{\dot{w}_0}\right] = 120 \qquad \dot{w}_0 = \frac{120}{1-\frac{1}{4^3}} = 121.9 \simeq \underline{\underline{122\ \tfrac{kg}{h}}}$$

$$W = 2\dot{w}_0\left[1 - \frac{1}{4^4}\right] = 2 \times 120\ \frac{1-\frac{1}{4^4}}{1-\frac{1}{4^3}} = 242.9 = \underline{\underline{243\ kg}}$$

Using the generalized equations presented here

$$I(R, R_0) = H(R - R_{min}) \qquad H(u) = \begin{cases} 0 & u<0 \\ 1 & u>0 \end{cases}$$

$$n_1(R) = \frac{\dot{w}_0}{W}\left(\frac{R}{R_0}\right)^3 \frac{1}{k}\ H(R - R_{min}) \qquad R_{min} \le R \le R_0$$

$$\dot{w}_0 - \dot{w}_2 = 120\ kg/h$$

Eq (A 4) gives
$$\frac{\dot{w}_2}{\dot{w}_0} = \left(\frac{R}{R_0}\right)^3$$

Eq (A1) gives
$$\frac{Wk}{\dot{w}_0 R_0} = \frac{1}{4}\left[1 - \left(\frac{R}{R_0}\right)^4\right]$$

These are the same as plug flow equations.

Cover AFR

Extensions to multi size feed, elutriation etc. are readily obtained

$$I(R,R_0) = \exp\left[-\int_{R_0}^{R} \frac{\dot{w}_1/W + \mathcal{K}(R)}{\mathcal{R}(R)}\,dR\right]$$

Let R_m be the smallest size in the feed
R_M be the largest size in the feed
$p_0(R)$ ~~dR~~ – fraction (mass) of particles of size R in feed

For growing particles:

$$\frac{W}{\dot{w}_0} = \int_{R_m}^{R(t\to\infty)} \frac{R^3}{|\mathcal{R}(R)|} I(R,R_m)\,dR \int_{R_m}^{R} \frac{p_0(R_i)\,dR_i}{R_i^3\, I(R_i,R_m)}$$

For shrinking particles

$$\frac{W}{\dot{w}_0} = \int_{R(t\to\infty}^{R_M} \frac{R^3}{|\mathcal{R}(R)|} I(R,R_M)\,dR \int_{R}^{R_M} \frac{p_0(R_i)\,dR_i}{R_i^3\, I(R_i,R_M)}$$

For growing particles

$$p_1(R) = \frac{\dot{w}_0 R^3}{W|\mathcal{R}(R)|} I(R,R_m^*) \int_{R_m}^{R} \frac{p_0(R_i)\,dR_i}{R_i^3\, I(R_i,R_m)}$$

For shrinking particles

$$p_1(R) = \frac{\dot{w}_0 R^3}{W|\mathcal{R}(R)|} I(R,R_M) \int_{R}^{R_M} \frac{p_0(R_i)\,dR_i}{R_i^3\, I(R_i,R_M)}$$

and

$$\dot{w}_1 + \dot{w}_2 - \dot{w}_0 = \int_{\text{all } R} \frac{3\, W\, p_1(R)\, \mathcal{R}(R)\, dR}{R}$$

Extensions to situations where gas composition varies in the reactor ~~———~~ can be made but are not as readily available in the literature.

Shrinking particles X 28a

Plug flow uniform gas composition

$$\frac{W}{F_0} = \int_0^{X_B} \frac{dX_B}{(-R_B)} \qquad \frac{dR}{dt} = -k$$

$$(-R_B) = \frac{4\pi R^2 \rho_B\left(-\frac{dR}{dt}\right)}{\frac{4}{3}\pi R^3 \rho_B} = \frac{3k}{R} = \frac{3\left(-\frac{dR}{dt}\right)}{R}$$

$$X_B = \frac{\frac{4}{3}\pi R_0^3 - \frac{4}{3}\pi R^3}{\frac{4}{3}\pi R_0^3} = 1 - \left(\frac{R}{R_0}\right)^3$$

$$dX_B = -\frac{3R^2}{R_0^3}\,dR \qquad \frac{W}{F_0} = \int_{R_0}^{R} \frac{R^3}{R_0^3\left(\frac{dR}{dt}\right)}\,dR$$

$$\frac{W}{F_0} = -\int_{R_0}^{R} \frac{3R^2 \cdot R}{R_0^3 \cdot 3k}\,dR = \frac{1}{\cancel{3}R_0^3 k}\int_R^{R_0} R^3\,dR$$

$$= \frac{1}{4R_0^3 k}\left[R_0^4 - R^4\right] = \frac{R_0}{4k}\left[1 - \left(\frac{R}{R_0}\right)^4\right]$$

But

$$\frac{dR}{dt} = -k \qquad R = R_0 - kt$$

$$t = 0 \quad R = R_0 \qquad \frac{R}{R_0} = 1 - \frac{k}{R_0}t$$

$$\boxed{\frac{W}{F_0} = \frac{R_0}{4k}\left[1 - \left(1 - \frac{kt}{R_0}\right)^4\right]}$$