Lecture 10

Fluidized Bed Reactors

This reactor type in which a bed of solids is suspended in a flowing gas (or liquid) stream was introduced in the early 1940’s. Fluidized bed reactors are particularly convenient devices for catalytic processing when catalyst life or stream is short and catalyst needs constant regeneration. Advantages fluidized beds are attractive for reaching rates not possible in fixed beds.

Fluidized bed reactors may operate in a variety of hydrodynamic regimes (see J. Chem. Eng. Data, 1978, p. 564):

- particulate fluidization
- bubbling regime
- chugging regime
- turbulent regime
- "fast bed" regime (clear dense fluidization)

One normally moves from one regime to the other as the superficial gas velocity is increased.

The typical pressure drop diagram is...
The formula for pressure drop at minimum fluidization results from a simple force balance

$$(-\Delta p_{mf}) = L_{mf} (1 - \varepsilon_{mf}) (p_b - p_g)$$  \hspace{1cm} (1)$$

$$(-\Delta p_{mf})$$ - pressure drop at minimum fluidization

$$L_{mf}$$ - bed length at minimum fluidization

$$\varepsilon_{mf}$$ - bed porosity (voidage) at minimum fluidization

$$p_b, p_g$$ - particle and gas mean density (appropriate)

Bed length at minimum fluidization

$$L_{mf}$$, porosity at minimum fluidization

$$\varepsilon_{mf}$$ are best determined experimentally using the parr还想 that interest end measured pressure drop data. From such measurements minimum fluidization velocity, $$u_{mf}$$, can be obtained also.

However, all of these quantities can also be predicted from correlations to a large or lesser degree empirically.

For voidage of minimum fluidization

$$\varepsilon_{mf} = \left\{ \frac{18 \sqrt{33.7}^2 + 0.0408 \text{ Ga} - 33.7}{2.70 \sqrt{33.7}^2 + 0.0408 \text{ Ga} - 33.7} \right\}$$

$$\text{Ga} = \frac{d_p}{\mu} \left( \frac{p_b - p_g}{p_b} \right)$$ - Galileo number

$$d_p = \left( \frac{6 \text{ Vp}}{\pi} \right)^{1/3}$$
This correlation underpredicts the exit by about 20% for spherical particles and is even less reliable for nonspherical particles. Experimentsally measured exit for a variety of solids vary from a low of 0.40 to a high of 0.60.

Bed height can be calculated from:

\[ L_{mf} = \frac{L_{fb}}{(1 - \varepsilon_b)} \left(1 - e_f\right) \]  

\[ W_s = \rho_b L_{fb} A_b = \rho_s L_{fb} (1 - \varepsilon_b) \]  

where \( L_{fb} \) = height of solids will no see flowing

\( A_b \) = cross sectional area of the bed

\( W_s \) = total mass of solids in the bed

\( \varepsilon_b \) = porosity of the fixed bed

\( \rho_b \) = bulk density of solids in bed (provided by catalyst manufacturers)

Predic bed height of open top conditions \( L_f \) requires the knowledge of porosity \( \varepsilon_f \) at open top conditions:

\[ L_f = \frac{L_{mf} (1 - \varepsilon_{mf})}{(1 - e_f)} \]

\[ \frac{U_0}{U_t} = \varepsilon_f^m \]  

\( U_0 \) = superficial gas velocity

\( U_t \) = terminal velocity

\( m \) = exponent to be determined experimentally.
Thus correct prediction of operating bed lengths requires the knowledge of bubble frequency of which alone but mainly due to presence of bubbles.

The bubble frequency per unit cross sectional area $v_b$ is known:

$$v_b = \alpha e^{-\beta h}$$  \hspace{1cm} (6)

where $\alpha$, $\beta$ are constants and $h$ is height coordinate in bed height. $L_f$ can be calculated:

$$L_f = \frac{6}{\beta} \ln \left\{ \left( \frac{1 + \frac{C}{u_b \sqrt{u_b}} e^{\frac{\beta L_f}{6}} - 1}{\frac{C}{u_b \sqrt{u_b}}} \right) \right\}$$  \hspace{1cm} (7)

where

$$C = 0.711 \left[ \left( \frac{6(u_b - u_m)}{\pi \alpha} \right)^{1/3} \right]^{1/2}$$  \hspace{1cm} (8)

Bed lengths can also be predicted (with accuracy of at least 30% or more) from the strictly empirical correlation of Frantz (Kansan to Campus Report):

$$\frac{L_f - L_{mf}}{L_{mf}} = 0.43 D^{-0.43} L_{mf}^{-0.2} u_m^{-0.035}$$  \hspace{1cm} (9)

$$m = 0.328 0.35 0.43 L_{mf} -0.25$$  \hspace{1cm} (10)

with $D$ (ft), $L_{mf}$ (ft), $\beta$ ($\alpha^{rac{1}{13}}$), $u_m$ (ft/s).

This correlation is embedded in Kansan to Campus program for fluidized bed design and should be viewed with caution.
Particle selectivity

For calculation of maximum fluidization velocity and pressure drop, it is necessary to define particle selectivity

\[ \psi = \left( \frac{\text{surface of value}}{\text{surface of particle of same size}} \right) = \frac{W}{2\pi} \left( \frac{6V_0}{W} \right)^{2/3} \]  \hspace{1cm} (11)

A measure of selectivity can be obtained from the following correlation:

\[ \psi = \left[ \frac{11}{1 - E_{mf}} \right]^{-2} \]  \hspace{1cm} (12)

Minimum fluidization velocity

The most popular correlation for prediction of minimum fluidization velocity is Krts of Law:

\[ U_{mf} = 1.118 \times 10^{-13} \frac{dp^{1.82} \left( s_2 - s_1 \right)^{0.34}}{\rho^{0.66} \mu^{0.88}} \]  \hspace{1cm} (13)

where \( U_{mf} \) (m/s), \( dp \) (μm), \( s \) (kg/m³), and \( \mu \) (Ns/m²).

This correlation, however, deviates often by too a factor of 2 or more from industrial data.

Instead, the extrapolation of the Ergun equation for packed beds is suggested:

\[ \frac{1.75}{\psi^{3/2}} \left( \frac{dp U_{mf} \rho_2}{\mu} \right)^2 + \frac{150(1-E_{mf}) \left( dp U_{mf} \rho_2 \right)}{\psi^2 E_{mf}^3 \left( \frac{dp \rho_2}{\mu} \right)^2} = \frac{dp \rho_2 (s_2 - s_1)}{\mu^2} \]  \hspace{1cm} (14)

In first approximating form:

\[ U_{mf} = \left( \frac{dp}{150} \right)^{2} \frac{p_2 - p_1}{\mu} s \left( E_{mf}^3 \right) \]  \hspace{1cm} (15a)

for \( Re_p \approx \frac{U_{mf} dp p_2}{\mu} < 20 \)

and
Limit \[ \text{Limit} = \left( \frac{\gamma \Delta p}{1.75 \frac{\rho - \rho_l}{\rho}} \right)^{1/2} \]  \hspace{1cm} (15b)

For \( R_e \geq 1000 \)

Using the previous estimates for \[ \Delta p \] of which are unknown one gets

\[ \text{Limit} = \frac{\Delta p^2 (\rho - \rho_l)}{1650 \mu} \] \hspace{1cm} (16a)

\[ \text{Limit} = \left( \frac{\Delta p (\rho - \rho_l)}{24.5 \mu} \right)^{1/2} \] \hspace{1cm} (16b) \hspace{1cm} \text{for} \ R_e > 1000 \]

For particles of varying size \( d_p \) should be replaced by the mean particle diameter \( d_p \) based on the equality of actual external particle area and area of "mean" nine pores.

\[ d_p = \frac{1}{\int_{d_p}^{d_p_{max}} p(d_p) \, dp} \] \hspace{1cm} (17)

\[ p(d_p) \, dp = \text{mass of particles of size } d_p \]

Mode of fluidization

It is important to assess in what regime will the fluidized bed operate. Viable fluidization velocities are constrained by minimum fluidization velocity and terminal particle settling velocity. Terminal velocity can be determined from:

\[ u_t = \left[ \frac{4 \, g \, \rho_p (\rho - \rho_l)}{3 \, \rho_l \, C_D} \right]^{1/2} \] \hspace{1cm} (18)

when \( C_D \) - drag coefficient is available.
optical and mass transfer optimization in terms of charts of \( C_D \) vs. \( \text{Re}_f \)

usually,

\[
10 \leq \frac{C_D}{\text{Re}_f} \leq 90 \quad \text{(19)}
\]

which thus the wide range of possible operating conditions for \( \text{Re}_f \) by violating bubbling limits it is possible to increase even further \( \text{Re}_f \) with only modest wall entrainment.

for predicting the mode of affection how the following criterion is suggested

\[
\text{Flat Repeat} \left( \frac{C_D - C_B}{C_B} \right) \left( \frac{\text{Len}_f}{D} \right) \leq 100 \quad \text{for bubble} \quad \text{(20)}
\]

\[
\text{Flat Repeat} \left( \frac{C_D - C_B}{C_B} \right) \left( \frac{\text{Len}_f}{D} \right) > 100 \quad \text{for bubbling}
\]

\[
\text{Flat} = \frac{\text{Un}_f^2}{\text{dp} \, j} \quad i \text{ bldg} = \frac{\text{dp} \, \text{Un}_f^2}{j}
\]

A Similicity parameter can be stated as:

\[
\frac{\text{dp} \, \text{Un}_f}{j} < 1 \quad \text{for bubble to absence in} \quad \text{(21)}
\]

\[
\frac{\text{dp} \, \text{Un}_f}{j} > 10 \quad \text{for bubbling}
\]

where \( \text{dp} \) is maximum bubble rise which is obtainable from a number of correlations.

Stagnation occurs if:

\[
\frac{\text{dp} \, \text{Un}_f}{j} \geq 800
g \left( \frac{\text{dp} \, \text{Un}_f}{j} \right) > 1 \quad \text{D} \leq 2 \text{} \text{dp} \, \text{Un}_f
\]

\[
\frac{C_D - \text{Un}_f}{0.35 \left( \text{g} \, D \right)^{1/2}} > 0.2 \quad \text{Stewart's column} \quad \text{(22)}
\]
Many additional calculations have to be made in fluidized bed reactor design regarding:
- maximum bubble diameter
- bubble rise velocity
- bubble rise distribution
- grid hole velocity
- bubble penetration at the grid
- transport dispersion aging height
- maximum particle rise entrainment rate
- entrainment rate
- minimum entrainment velocity
- rate of gas hole attachment
- electronegative constants
- gas-pore hole heat transfer coefficients
- gas backmixing
- solids backmixing
- heat transfer coefficients to the wall
- heat transfer to horizontal, vertical, tubes, coils

We will not dwell on these here but will concentrate on modeling aspects of fluidized bed reactors.

We refer to excellent texts and papers covering the topics mentioned above. The most outstanding sources are:
Maximum Bubble Rise

Since fluidization regime depends on maximum bubble rise, we can use some simple ways of approximating that parameter.

Davidson-Harman model concludes that bubbles rise slowly if:

\[ U_{cr} \leq U_f \]

\[ 0.711 \left( \frac{g \rho_d}{3 \rho_f} \right)^{1/2} \leq \left[ \frac{4 g \rho_d (\rho_f - \rho)}{3 \rho \rho_f} \right]^{1/2} \]

\[ d_{max} = \frac{4 \rho \rho_f (\rho_f - \rho)}{3 (0.711)^2 \rho_f \rho \rho_f} \]

An alternative formula is:

\[ \frac{d_{max}}{d_p} = 7.3 \left( \frac{A^2}{g \rho_d \rho_f^2} \right) \left[ \frac{\rho_f - \rho}{1 - \rho_f} \right] \left[ \left( 1 + \frac{2 g \rho^3}{5 \rho_f^3 (\rho_f - \rho)} \right)^{1/2} - 1 \right] \]

An average bubble diameter is estimated from bed expansion:

\[ d_b = \frac{1}{4} \left( \frac{L_{avg}}{L - L_{avg}} - 0.711 \right) \]

Bubble rise control by internals

Vertical heat exchanger tubes. Effective control does not interfere with solids recirculation.

\[ d_e = 4 \left( \frac{\text{cross section of bed}}{\text{wetted perimeter}} \right) \]

Horizontal heat exchanger tubes or baffles.

Unpredictable effect on bubble rise, in bypass in solid circulating beds.
Cold Modeling

Modelling the hydrodynamics of fluidized beds by observing the phenomena in scaled-down cold models is of great interest. It has been shown that the scale-up or scale-down should be based on the following four dimensionless groups:

- \( \frac{P}{\rho g} \); ratio of solids to gas density
- \( \frac{d_p}{L} \); ratio of particle size to a characteristic bed dimension
- \( \frac{u^2}{\rho g} \); ratio of superficial gas velocity
- \( \frac{d_p u}{\rho g} \); Scaled to the product of acceleration of gravity and characteristic bed dimension

\[ \frac{d_p \rho g}{\mu} \]; fan hole Reynolds number

It has been documented via movies that when the above four dimensionless groups are identical, the bubble's behavior of the beds is identical. Thus, a behavior of a Sand/R12 green model can be simulated by a cork/air system. Similarly, an expanded polystyrene/air system can be used to simulate a transfer capacity water system.

The viability of cold modeling still needs further confirmation by for models with wide fan hole size distribution since all the experiments do not deal with narrow fan hole size distribution.
Modeling of Catalytic Fluidized Bed Reactors

All models consider the bed to consist of two or more "pseudo" phases: bubble phase, emulsion phase, cloud phase, etc. The simplest models consist of only bubble and emulsion phase. In the models it is usually assumed that the bubble rise velocity is given by:

$$u_b(1-\epsilon_f) = u_{br}(1-\epsilon_f)$$  \hspace{1cm} (1)$$

or:

$$u_b = u_p - u_{mf} + u_{br}$$ \hspace{1cm} (2)$$

$$u_p = \frac{Q_g}{A_R}$$ \hspace{1cm} (3)$$

$$u_{br} = 0.711 \left( \frac{\rho_d}{\rho_b} \right)^{1/2}$$ \hspace{1cm} (4)$$

The above is based on the assumption that all the gas flow in addition to the one required for minimum fluidization passes through the bed in terms of bubbles.

Hey-Wa Debooter Model

Assumptions:
- bubble phase in plug flow
- axial dispersion model applicable to emulsion phase
- no catalyst in bubble phase

$$f_b \ u_b \ \frac{dC_{ab}}{dz} + K_I (C_{ab} - C_{ae}) = 0$$ \hspace{1cm} (5)$$

$$f_e \ u_e \ \frac{dC_{ae}}{dz} - f_e D_e \ \frac{d^2C_{ae}}{dz^2} - K_I (C_{ab} - C_{ae}) + \beta_{ae} \epsilon_e (1-f_b) = 0$$ \hspace{1cm} (6)$$
\[ z = 0 \quad C_{b0} = C_{a0} \quad \text{(7a)} \]
\[ -D_e \frac{dC_a}{dz} = u_e (C_{a0} - C_a) \quad \text{(7b)} \]
\[ z = L_f \quad \frac{dC_a}{dz} = 0 \quad \text{(8)} \]

\[ K_i \left( \frac{m^3}{m^3 \text{ bed h}} \right) \quad \text{exchange (interchange) coefficient between bubble and emulsion phase} \]

\[ \rho_b \left( \frac{m^3 \text{ bubbles}}{m^3 \text{ bed}} \right) \quad \text{bubble holding} \]

\[ \rho_e \left( \frac{m^3 \text{ gas in emulsion}}{m^3 \text{ bed}} \right) \quad \text{gas holdup in emulsion phase} \]

\[ \rho_c \left( \frac{kg \text{ catalyst}}{m^3 \text{ gas in emulsion}} \right) \quad \text{catalyst mass in emulsion phase} \]

\[ u_b, u_e \left( \frac{m}{s} \right) \quad \text{bubble and emulsion phase velocity, respectively} \]

\[ \text{Raw} \left( \frac{m^3 \text{ catalyst}}{m^3 \text{ bed h}} \right) \quad \text{rate of reaction for unit mass of catalyst} \]

The exit gas concentration is given by:

\[ u_0 C_a = u_b \rho_b C_{b0} (L_f) + u_e \rho_e C_{a0} (L_f) \quad \text{(9)} \]

The model can be further simplified by assuming plug flow, \( D_e \to 0 \), or stirred tank behavior, \( D_e \to \infty \), for the emulsion phase. Otherwise, \( D_e \) must be determined from correlations based on fluid shear:

\[ \frac{u_0 L_f}{D_e} (D/P)^{15/2} = 0.3 \quad \text{for } \frac{u_0}{u_{	ext{jet}}} \leq 0.75 \quad \text{(10)} \]

Similarly, the interchange coefficient can be found from correlations:

\[ \frac{u_0}{K_i} = 1.5 \frac{L_f}{D} 0.42 \quad \text{for } \frac{u_0}{u_{	ext{jet}}} = 15 \quad \text{(11)} \]
\[ \theta = \frac{\theta_0 - \theta_{eq}}{\theta_f} \quad (12) \]

\[ \theta_c = \theta_f - \theta_b \quad (12) \]

\[ \theta_c = \theta_{eq} \quad \Rightarrow \quad \theta_c = \frac{P_0(1-k)\theta_f}{\theta_f + k} \quad (14) \]

Van derkuis's model seems to hold well for first order reactions and relatively low Damköhler numbers (slow reactions)\[ k < 3 \left( \frac{m^3}{kg \text{cat h}} \right). \]

Predictions of the model based on various degrees of backmixing and exchange are sketched below for a first order system.

**Conclusions**
- Pseudo-homogeneous models of a PFR & CSTR do not provide trends or reactor performance.
- Degree of backmixing in exchange is important than exchange coefficient.
- At low exchange coefficients, one may have worse performance than in a CSTR.
The following discussion is based on the results of the experiment described above. The values obtained agree closely with the theoretical predictions. The accuracy of the measurements was within 5%. The data were analyzed using statistical methods to ensure the reliability of the results. Further experiments are planned to verify these findings.
\[
\begin{align*}
\frac{y_b}{u_b} \frac{dC_b}{d\tau} + K_{bc} (C_b - C_a) + \frac{k_W y_b}{\gamma_b} \rho_s C_b &= 0 \quad (15) \\
K_{bc} (C_a - C_b) - k_W \gamma_c \rho_s C_a - K_{ce} (C_a - C_c) &= 0 \quad (16) \\
K_{ce} (C_a - C_e) - k_W \gamma_e \rho_s C_e &= 0 \quad (17) \\
\tau = 0 \quad C_b = C_a \quad (18)
\end{align*}
\]

where:
\[
K_{ce} = \frac{K_{ce} A_c e}{A_b}, \quad K_{bc} = \frac{k_{bc} A_c}{A_b}
\]
\[
\gamma_b = 1 - \varepsilon_b', \quad \gamma_e = \frac{(1 - \varepsilon_e') A_e}{A_b}
\]

The rate of reaction was given as
\[
-R_A = k_W C_A \left( \frac{k_W y_b}{\gamma_b} \rho_s + s \right)
\]

The exit bubble concentration is given by:
\[
\ln \left( \frac{C_a}{C_b(0)} \right) = \left[ \frac{k_W y_b \rho_s + \frac{1}{K_{bc}} + \frac{1}{k_W \rho_s C_b + \frac{1}{K_{ce} + k_W \rho_s e}}} \right] \frac{L}{u_b}
\]

or
\[
\ln \left( \frac{C_a}{C_b(0)} \right) = K_r \frac{L}{u_b}
\]

---

very slow reactions: very poor performance

very fast reactions: very poor performance

\( K_r \) defined by brackets above
This equation can also be written as:

\[ \ln \left( \frac{C_{a0}}{C_{a}(t)} \right) = K_r \frac{u_p}{(1 - \epsilon_f)} \frac{W}{u \epsilon_f P_f} \quad (20.6) \]

where: \( W \) - mass of catalyst in bed
\( \epsilon_f \) - volume fraction of gas flow rate

Model applicable to bubbling regime, fast bubble!

Example: Let us illustrate the application of the above model with the following example.

\[ A \rightarrow R \quad \text{(first order)} \]

Reaction rate: \( k \) \( A \rightarrow R \) \( k = 4 \times 10^{-4} \text{ m}^3/\text{kg cat} \text{ s} \)

Gas velocity: \( u_g = 0.3 \text{ m/s} \)

Minimum fluidization condition: \( u_{mf} = 0.03 \text{ m/s} \)

\( \epsilon_f = 0.5 \)

Bed diameter: \( D = 2 \text{ m} \)

Bed mass: \( W = 7000 \text{ kg catalyst} \)

Catalyst density: \( \rho_s = 2000 \text{ kg/m}^3 \)

Bubble size: \( d_B = 0.32 \text{ m} \)

Feed catalyst: \( C_{a0} = 100 \text{ mol/m}^3 \)

Diameter: \( D = 2 \times 10^{-5} \text{ m/s} \)

Fraction of make to bubble volume: \( \epsilon_f = 0.33 \)

\( \epsilon_f < 0.5 \) check model applicability

Bubble rise velocity (single bubble in bed at \( \epsilon_f \))

\[ u_{b0} = 0.711 (9.8 \times 0.32) = 1.26 \text{ m/s} \]

\[ \frac{u_{b0}}{u_{mf}} = \frac{1.26}{0.03/0.5} = 21 \]

Bubbling bed model is valid

Calculate:

Bubble rise velocity,

\[ u_b = u_{b0} - u_{mf} + u_{mf} = 0.30 - 0.03 + 1.26 = 1.53 \text{ m/s} \]
Estimate bed voidage:
\[ \varepsilon_b = 1 - \frac{u_{mf}}{u_b} (1 - \varepsilon_f) = 1 - \frac{0.26}{0.33} (1 - 0.5) = \]

Calculate bed fraction in bubbles:
\[ \delta = \frac{u_p - u_{mf}}{u_b} = \frac{0.3 - 0.03}{0.33} = 0.177 \]

Calculate bubble - cloud exchange coefficient:
\[ K_{bc} = 4.50 \left( \frac{u_{mf}}{u_b} \right) + 5.85 \left( \frac{0.14 \times 0.14}{0.33} \right) = 4.5 \left( \frac{0.03}{0.32} \right) + 5.85 \left( \frac{2 \times 10^{-5}}{0.32} \right) \]
\[ K_{bc} = 0.61 \text{ (s}^{-1} \text{)} \]

Calculate cloud - eumalic exchange coefficient:
\[ K_{ce} = 6.78 \left( \frac{E_{mf} \delta u_b}{u_b^3} \right)^{1/2} = 6.78 \left( \frac{0.5 \times 2 \times 10^{-5} \times 0.33}{0.32^3} \right) = 0.147 \text{ (s}^{-1} \text{)} \]

Estimate fraction of voids in bubbles:
\[ \varepsilon_b = 0.03 \left( \frac{m^3 \text{ solids}}{m^3 \text{ bubbles}} \right) \Rightarrow \text{really does not have an effect on evaporation} \]

Calculate fraction of voids in clouds:
\[ \varepsilon_c = (1 - \varepsilon_{mf}) \left[ \frac{3 u_{mf}/E_{mf}}{u_b - u_{mf}/E_{mf}} \right] = \]
\[ = (1 - 0.5) \left[ \frac{3 \times 0.03/0.5}{1.26 - 0.03/0.5 + 0.33} \right] = 0.24 \left( \frac{m^3 \text{ solids}}{m^3 \text{ cloud}} \right) \]

Calculate fraction of voids in eumalic
\[ \varepsilon_e = \left( \frac{1 - \varepsilon_{mf}}{\varepsilon_f} - \varepsilon_c \right) - \varepsilon_b = \frac{(1 - 0.5)(1 - 0.177)}{0.177} - 0.24 - 0.003 \]
\[ \varepsilon_e = 2.09 \left( \frac{m^3 \text{ solids}}{m^3 \text{ eumalic}} \right) \]

\[ k_p = 4 \times 10^{-4} \times 2 \times 10^{-3} = 0.8 \text{ (1/s)} \]

\[ k_r = \left[ \frac{n_{\text{heterotrope}}}{0.8 \times 0.003} + \frac{1}{0.614 + \frac{1}{0.8 \times 0.24 + \frac{1}{0.147 \delta / 0.109}}} \right] = 0.216 \]
\[
\frac{\frac{W}{Q_0}}{(1-0.5) \times 1.26 \times 2000} = \frac{7000}{\pi \times 1 \times 0.3} = 1.77
\]

\[
\ln \frac{C_{ao}}{C_{ao}(t)} = 0.38
\]

\[
\frac{C_{ao}(t)}{C_{ao}} = 0.68
\]

\[
x_4 = 0.32
\]

In a fixed bed reactor (plug flow behavior) using the same amount of catalyst (or recycle if one with some effectiveness factor), conversion would be:

\[
\frac{\ln C_{ao}}{C_{ao}/\hat{C}_{per}} = \frac{kW}{Q_0} = \frac{4 \times 10^{-4} \times 7 \times 10^3}{\pi \times 1 \times 0.3} = 2.97
\]

\[
\frac{\hat{C}_{per}}{C_{ao}} = 0.05
\]

\[
x_{appr} = 0.95
\]

If gas were in completely backmixed state (CSTR - ideal tank behavior)

\[
\frac{C_{ao} x_{acstr}}{kW (1-x_{acstr})} = \frac{W}{Q_0}
\]

\[
x_{acstr} = \frac{1}{1 + \frac{kW}{Q_0}} = \frac{1}{1 + 4 \times 10^{-4} \times 7 \times 10^3} = 0.75
\]

\[
x_{acstr} = 0.75
\]

The solids in the accumulator are stored off the gaseous reactant, and most of the gas dissolves through the bubbles.
Slugging Bed Reactors

Often in laboratory scale one is forced to use small diameter beds with \( L_b/D > 1 \), in which slugging is almost inevitable.


The following steps should be taken:

a) Calculate

\[
\frac{u_0 - u_{mf}}{0.35 (g D)^{1/2}}
\]

If this parameter is greater than 0.2 and \( L_f/D > 1 \) then flow will occur.

The criterion may fail when most of the particles are less than 50 \( \mu \)m.

b) Estimate slug length, \( L_s \)

\[
\frac{L_s}{D} = 0.495 \left( \frac{L_s}{D} \right)^{1/2} \left[ 1 - \frac{u_0 - u_{mf}}{0.35 (g D)^{1/2}} \right] + 0.061 - \frac{1.939(u_0 - u_{mf})}{0.35 (g D)^{1/2}} = 0
\]

c) Calculate the transfer factor \( X \)

\[
X = \frac{R_b L_f}{u_{so} V_s} = \frac{(Rate \ of \ gas \ exchange \ between \ bed \ and \ environment \ per \ unit \ area \ per \ unit \ time) \times (Red \ length)}{(Rate \ of \ gas \ mixing \ per \ unit \ volume \ per \ unit \ length) \times (Volume \ of \ bed)}
\]

\[
\frac{u_{so} = k(4 - u_{mf}) + 0.35 (g D)^{1/2}}{4 \pi} \quad k = 1
\]

d) \( X = \frac{L_{mf} F_b}{0.35 (g D)^{1/2} D (F_b + u_{mf} F_p)} \left[ U_{mf} + 0.64 (D) \left( \frac{D}{2} \right)^{1/2} \right] \]

Where

Reduction factor \( \frac{F_b}{2 I_b} = \frac{\sqrt{m} D}{4 \pi D^2} \)

\( I_b = \int_{u_{mf}}^{\sqrt{2} U_{mf}} e^{-\gamma^2} d\gamma \)

Shake factor \( D = \frac{L_s}{D} - 0.495 \left( \frac{L_s}{D} \right)^{1/2} + 0.061 = \frac{4 V_s}{\pi} \)
\[ F_p = \sqrt{\frac{n}{e}} \frac{y_{in}^2}{k_1 \sqrt{b_2}} \]

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<th>( \frac{L}{D} )</th>
<th>0.3</th>
<th>0.5</th>
<th>1.0</th>
<th>2.0</th>
<th>3.0</th>
<th>4.0</th>
<th>5.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I )</td>
<td>0.13</td>
<td>0.21</td>
<td>0.35</td>
<td>0.71</td>
<td>0.98</td>
<td>1.24</td>
<td>1.48</td>
</tr>
</tbody>
</table>

\( D_g \) – gas diffusivity

Define Damkohler number for first order reaction

\[ Da = \frac{K_e \text{ Lmt \& Emt}}{u_0} = \frac{k \text{ Lmt}}{u_0} \]

\( K_e \) – first order reaction rate constant based on inorganic volume

\( K \) – first order reaction rate constant based on particulate phase volume

The above expression includes two bulk flow and diffusion contributions to the exchange coefficient. However, the formula gives an upper estimate for \( X \) especially in case of fast reactions.

\( Da > 20 \)

An approximate formula is useful especially in cases of smaller particles which view only exchange by diffusion.

\[ \frac{L_{mt}}{0.35(gD)^{1/2}D_{2/3}} \left[ \text{Unf} + 16 \text{Euf} \left( \frac{2}{n} \right) \left( \frac{g}{D} \right)^{1/4} \right] \]

The two equal for \( X \) identical for \( \text{dp} < 75 \mu m \).
d) Conversion for first order catalytic reaction can be obtained from:

\[ x_A = 1 - \frac{1}{r_1 - r_2} \left[ r_1 e^{-r_2 L (1 - \frac{L u_{mc}}{u_0})} - r_2 e^{-r_1 L (1 - \frac{L u_{mc}}{u_0})} \right] \]

where \( r_1, r_2 \) are roots of:

\[ 2L \frac{u_{mc}}{u_0} x_{1/2} = X + Da \pm \left[ (X + Da)^2 - 4Da \frac{u_{mc}}{u_0} \right]^{1/2} \]

where \( X \) is maximum height of the packing layer.

\[ L f \frac{L_{mc}}{L_{mf}} = \frac{u_0 - u_{mf}}{u_{mf} - \frac{0.35 (gD)^{1/2}}{}} \]

The model forugging bed reactors should be extended to gas-solid microcatalytic reactors. This, to my knowledge, has not been done.
Modeling of Aerosol-Flow 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 only.

\[
\dot{w}_1 \quad \text{(kg)} \quad \text{mass flow rate of the carryover stream}
\]

\[
\dot{w}_0 \quad \text{(kg)} \quad \text{mass of fluidized bed}
\]

Total feed rate of solids

\[
\dot{w}_1 \quad \text{(kg)} \quad \text{mass flow rate of the feedflow stream}
\]

\[
\dot{w}_1 + \dot{w}_2 > \dot{w}_0 \rightarrow \text{Particle growth}
\]

\[
\dot{w}_1 + \dot{w}_2 < \dot{w}_0 \rightarrow \text{Particle shrinkage}
\]

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

\[
0 = \dot{w}_0 \rho_0(R) - \dot{w}_1 \rho_1(R) - \dot{w}_2 \rho_2(R) - W \left[ \frac{d}{dr} \left( \rho_1(R) \frac{d}{dr} R \right) \right] + \frac{3W}{R} \rho_1(R) R^2
\]

\[
\rho_1(R) \text{d}R \quad \text{mass fraction of solids in the interval between } R \text{ and } R + \text{d}R
\]

\[
\rho_0(R), \rho_1(R), \rho_2(R) \quad \text{mass fractions describing particle size distribution in the feed, bed, and underflow and}
\]
overflow stream, describing

\[ R(k) = \left\{ \begin{array}{ll}
-k' \\
-k' k''
\end{array} \right. \]

particle shape

\[ R(k) = \left\{ \begin{array}{ll}
k' \\
k' k''
\end{array} \right. \]

particle grow K

In the above a uniform gas composition is assumed in the bed.

\[ K(k) \left( \text{s}^{-1} \right) \text{ electric in constant flow} \]

for nuclei of size \( k \)

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

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

\[ K^* \left( \frac{2}{\text{cm}^2 \text{ s}} \right) \text{ depends on void size} \]

Also

\[ \frac{dW(R)}{dt} = K W(R) \]

\[ K^* = \frac{K W}{A_t} \]

\[ \frac{\gamma^* dp}{\mu} \frac{1}{(u_0 - u_k)^2} \text{ VS } \frac{dp_{lim}}{\mu} \text{ available} \]

Better to take data on system of
For a single wire feed of powder to the reactor, the weight distribution can be described by the integral:

\[
\frac{W}{W_0} = \int_{R_0}^{R_{\infty}} \frac{R^3}{R(R)R_0^3} I(R,R_0) \, dR \quad (A1)
\]

where

\[
I(R,R_0) = \exp \left[ -\int_{R_0}^{R} \frac{\dot{W}_s}{\dot{W}} + \chi(R) \, dR \right] \quad (A2)
\]

The wire distribution in the bed is

\[
P_1(R) = \frac{\dot{W}_0}{W_0} \frac{R^3}{R_0^3} I(R,R_0) \quad (A3)
\]

Overall balance gives

\[
\dot{W}_1 + \dot{W}_2 - \dot{W}_0 = \int_{R_{\infty}}^{R_0} \frac{3W}{R} P_1(R) R(R) \, dR \quad (A4)
\]

\[
P_2(R) = \frac{W}{\dot{W}_2} \chi(R) P_1(R) \quad (A5)
\]

**Example 1:** We want to produce 150 kg/h of Si. In a fluidized bed, Si wire \( \dot{W}_0 = \mathrm{Si} + 2\mathrm{H}_2 \)

Seed particles of \( R = 100 \mu\text{m} \) are fed into the reactor. We want to produce a surface membrane particle size of \( R_s = 1000 \mu\text{m} \). The growth rate is \( 100 \mu\text{m/h} \).

Find the size of the reactor \( W \), and seed feed rate \( \dot{W}_1 \).
First recall that
\[ m_1(R) dR = \text{mass fraction of solids in the bed} \]
\[ m_1(R) dR = \frac{W \phi(R) dR}{N \frac{4}{3} \pi R^3 \rho_s} \]

The mass fraction of solids in the bed between \( R \) & \( R + dR \) is:
\[ m_1(R) dR = \frac{W \phi(R) dR}{N \frac{4}{3} \pi R^3 \rho_s} \]

Mean particle radius based on external surface is defined by:
\[ S_{ext} = N \frac{4}{3} \pi R_s^2 = N \int_{R_{min}}^{R_{max}} 4 \pi R^2 m(R) dR = \frac{3W}{R_s} \int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R} \]

\[ V = N \frac{4}{3} \pi R_s^3 = N \int_{R_{min}}^{R_{max}} \frac{4}{3} \pi R^3 m(R) dR = \frac{W}{R_s} \int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R} \]

\[ \frac{S_{ext}}{V} = \frac{3}{R_s} = \frac{3W}{R_s} \int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R} \]

\[ R_s = \frac{1}{\int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R}} \]

- Size of an hole whose surface to volume ratio equals that of all solids in the mixture.

Other averages can be defined:
\[ R_w = \frac{1}{\int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R^2}} \Rightarrow \text{weight average particle radius} \]
\[ R_w = \frac{1}{\int_{R_{min}}^{R_{max}} \frac{m(R) dR}{R^2}} \Rightarrow \text{weight average particle radius} \]

\[ \text{average of all } R_w \text{ of all } \text{particles in the mixture} \]
Let us solve the problem:

From (A2)

\[ I(R, R_0) = e^{-\frac{R}{KW}(R_0 - R)} \]

Since \( R(R) = k = 100 \text{ mm/h} \)

From (A3)

\[ P(R) = \frac{\dot{w}_0}{Wk} \frac{R^3}{R_0^3} e^{\frac{\dot{w}_i}{KW}(R_0 - R)} \quad \text{for} \ R > R_0 \]

From (A4)

\[ \frac{\dot{w}_i}{\dot{w}_0} = 1 + \int_0^{R_0} \frac{3 \dot{w}_0}{R_0^3} e^{\frac{\dot{w}_i}{KW} R} R^2 e^{-\frac{\dot{w}_i}{KW} R} dR \]

\[ \frac{\dot{w}_i}{\dot{w}_0} = 1 + 3 \frac{Wk}{\dot{w}_i R_0} + 6 \left( \frac{Wk}{\dot{w}_i R_0} \right)^2 + 6 \left( \frac{Wk}{\dot{w}_i R_0} \right)^3 \]

\[ \bar{R}_s = \frac{1}{\frac{\dot{w}_0}{Wk R_0^3} e^{\frac{\dot{w}_i}{KW} R_0} \int_0^{R_0} R^2 e^{-\frac{\dot{w}_i}{KW} R} dR} = \frac{1}{\frac{\dot{w}_0}{Wk R_0^3} e^{\frac{\dot{w}_i}{KW} R_0} \left[ -R^2 \frac{KW}{\dot{w}_i} e^{-\frac{\dot{w}_i}{KW} R} - 2R \left( \frac{KW}{\dot{w}_i} \right)^2 e^{-\frac{\dot{w}_i}{KW} R} - 2 \left( \frac{KW}{\dot{w}_i} \right)^3 e^{-\frac{\dot{w}_i}{KW} R} \right]} = \frac{Wk}{\dot{w}_0} \left[ \frac{KW}{\dot{w}_i R_0} + 2 \left( \frac{KW}{\dot{w}_i R_0} \right)^2 + 2 \left( \frac{KW}{\dot{w}_i R_0} \right)^3 \right] = 3 \frac{Wk}{\dot{w}_0} \frac{\dot{w}_i}{\dot{w}_0} - 1 \]

\[ \bar{R}_s = \frac{3 Wk / \dot{w}_0}{\dot{w}_i / \dot{w}_0} - 1 \]
Example 2: We are producing TCS in a fluidized bed.

\[ \text{Si}(s) + \text{H}_2(g) + 3\text{SiCl}_4(g) = 4\text{SiCl}_2\text{H}_3(g) \]

The solids feed consists of a single particle one. \( d_0 = 200 \mu m \). These particles under reheat conditions would react completely in 8 h. However, the particles shrink to 50 \( \mu m \) 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 shrinking:

\[ R(t) = -kt \]

\[ \frac{R_0 - R}{k} = t \]

\[ R_0 - R = kt \]

\[ k = \frac{R_0 - R}{t} = \frac{200 - 50}{8} = 25 \mu m/h \]

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

\[ \bar{t} = \frac{R_0 - R_{inin}}{k} = \frac{200 - 50}{25} = 6 (h) \]

Last time (lecture 9) we developed the equation for the flow of solids and the constant shrinking rate:

\[ \frac{Wk}{W_0 d_0} = \frac{1}{4} \left[ 1 - \left( \frac{R}{R_0} \right)^4 \right] = \frac{1}{4} \left[ 1 - \left( 1 - \frac{kt}{R_0} \right) \right] \]

For the current example:

\[ \frac{25 W}{200 W_0} = \frac{1}{4} \left[ 1 - \left( \frac{50}{200} \right)^4 \right] \]

\[ \frac{W}{W_0} = 2 \left[ 1 - \frac{1}{4\bar{t}} \right] \]
At the same time since the number of particles in the feed and diluted stream is the same:

\[
\frac{\dot{w}_2}{\dot{w}_0} = \left(\frac{R}{R_0}\right)^3 = \left(\frac{50}{200}\right)^3 = \frac{1}{43}
\]

We want to use 120 lb/hr of Si, i.e.,

\[
\dot{w}_0 - \dot{w}_2 = 120
\]

\[
\dot{w}_0 \left[1 - \frac{\dot{w}_2}{\dot{w}_0}\right] = 120
\]

\[
\dot{w}_0 = \frac{120}{1 - \frac{1}{43}} = 121.9212243
\]

\[
W = 2\dot{w}_0 \left[1 - \frac{1}{43}\right] = 2 \times 120 \left[1 - \frac{1}{43}\right] = 242.9 = 243 \text{ kg}
\]

Using the generalized equations presented here,

\[
I(R, R_0) = H(R - R_{cm})
\]

\[
H(u) = \begin{cases} 0 & u < 0 \\ 1 & u > 0 \\ 1 & u = 0 \\ \frac{1}{4} & u < 0
\end{cases}
\]

\[
M(R) = \frac{\dot{w}_0}{-\dot{w}} \left(\frac{R}{R_0}\right)^3 \frac{1}{k} \cdot H(R - R_{cm})
\]

\[
\dot{w}_0 - \dot{w}_2 = 120 \text{ lb/hr}
\]

\[
\text{Eq. (A4) gives } \frac{\dot{w}_2}{\dot{w}_0} = \left(\frac{R}{R_0}\right)^3
\]

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

These are the same as any flow equations.
Extensions to multi nice feed, ebbrichs, etc. are readily obtained.

\[ I(R, R_0) = \exp \left[ -\int_{R_0}^{R} \frac{W_i}{W + \Delta W} \frac{dR}{W(R)} \right] \]

Let \( R_m \) be the smallest nice to be fed.

\( R_m \) be the largest nice to be fed.

\( \rho_0(R) \, dR \) the mass of particles of nice \( R \) in feed.

For growing particles:

\[ \frac{W}{\bar{W}_0} = \int_{R_m}^{R} \frac{R^3}{W(R)} I(R, R_m) \, dR \int_{R_m}^{R} \frac{\rho_0(R_i) \, dR_i}{R_i^3 \, I(R_i, R_m)} \]

For shrinking particles:

\[ \frac{W}{\bar{W}_0} = \int_{R_0}^{R_m} \frac{R^3}{W(R)} I(R, R_m) \, dR \int_{R}^{R_m} \frac{\rho_0(R_i) \, dR_i}{R_i^3 \, I(R_i, R_m)} \]

For growing particles:

\[ \rho_1(R) = \frac{\bar{W}_0 \, R^3}{W(R)} I(R, R_m) \int_{R_m}^{R} \frac{\rho_0(R_i) \, dR_i}{R_i^3 \, I(R_i, R_m)} \]

For shrinking particles:

\[ \rho_1(R) = \frac{\bar{W}_0 \, R^3}{W(R)} I(R, R_m) \int_{R}^{R_m} \frac{\rho_0(R_i) \, dR_i}{R_i^3 \, I(R_i, R_m)} \]

\[ \dot{W}_1 + \dot{W}_2 - \dot{W}_0 = \int_{R}^{R_m} 3 \, \frac{\nu \rho_1(R) \, R^2 \, dR}{W} \]

Extensions to other has where gas composition varies in the reactor can be made, but are not as readily available as the limiting case.