April 6, 2005: Chemical reactors, porous media

Recall results for plug flow, perfect mixing:

- Plug flow: homogeneous $C_A/C'_A = \exp(-kV/Q)$, heterogeneous $C_A/C_{A0} = \exp(-k''A/Q)$.
- Perfect mixing: homogeneous $C_A/C'_A = 1/(1+kV/Q)$, heterogeneous $C_A/C_{A0} = 1/(1+kA/Q)$.

How to tell whether plug or mixed? Tracers, Peclet number (more details in the slides).

Porous Media Darcy's Law for seeping flow through a medium:

$$Q = \frac{k_D A \Delta P'}{L} \tag{4.89}$$

($\Delta P'$ includes Δp and gravity), where k_D is the permeability. For a given geometry, we can define specific permeability $\mathcal{P}$ as:

$$k_D = \frac{\mathcal{P}}{\mu}. \tag{4.90}$$

The superficial velocity V_0 is then given by:

$$V_0 = \frac{Q}{A} = -\frac{\mathcal{P}}{\mu}\left(\frac{\partial P}{\partial x} - \rho g\right) \tag{4.91}$$

Tube bundle approximation: average velocity in the pores with volume fraction ω is:

$$\bar{V} = \frac{V_0}{\omega}. \tag{4.92}$$

Then define the hydraulic radius R_h for a fluid volume V_h with wetting surface area A_w as:

$$R_h = \frac{V_h}{A_w}. \tag{4.93}$$

For a porous solid of wetting surface area/total volume ratio S, it's usually useful to define the surface area/solid volume ration S_0 as

$$S_0 = \frac{S}{1-\omega}. \tag{4.94}$$

Then the hydraulic radius becomes:

$$R_h = \frac{V_h/V}{A_w/V} = \frac{\omega}{S} = \frac{\omega}{S_0(1-\omega)}. \tag{4.95}$$

Remember the Hägen-Poisseuille equation:

$$Q = \frac{\pi(P_1 - P_2)}{2\mu L}\left[\frac{R^2 r^2}{2} - \frac{r^4}{4}\right]_0^R = \frac{\pi(P_1 - P_2)R^4}{8\mu L}. \tag{4.96}$$

And average velocity:

$$u_{av} = \frac{Q}{A_{xs}} = \frac{\frac{\pi(P_1-P_2)R^4}{8\mu L}}{\pi R^2} = \frac{(P_1 - P_2)R^2}{8\mu L}. \tag{4.97}$$

Now relate this back to V_0 and R_h:

$$\bar{V} = K_1 \frac{\Delta P' R_h^2}{L\mu};\ V_0 = K_1 \frac{\Delta P' R_h^2 \omega}{L\mu}. \tag{4.98}$$

And substituting R_h:

$$V_0 = K_1 \frac{\nabla P' \omega}{L\mu} \frac{\omega^2}{S_0^2 (1-\omega)^2}. \tag{4.99}$$

This is the Blake-Kozeny equation.

Relate this back to the Darcy equation:

$$Q = \frac{\mathcal{P}}{\mu} \frac{A \Delta P'}{L} \Rightarrow V_0 = \frac{\mathcal{P} \Delta P'}{\mu L}. \tag{4.100}$$

This gives an expression for $\mathcal{P}$:

$$\mathcal{P} = K_1 \frac{\omega^3}{S_0^2 (1-\omega)^2}. \tag{4.101}$$

Note that for packed beds, $K_1 \simeq 1/4.2$.

Now beyond laminar flow, need a f-Re correlation. Define the Reynolds number:

$$\mathrm{Re} = \frac{\rho \bar{V} R_h}{\mu} = \frac{\rho V_0}{\mu (1-\omega) S_0}, \tag{4.102}$$

Later we'll relate this to a friction factor.