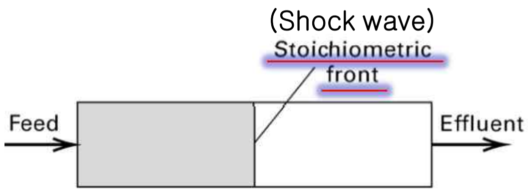
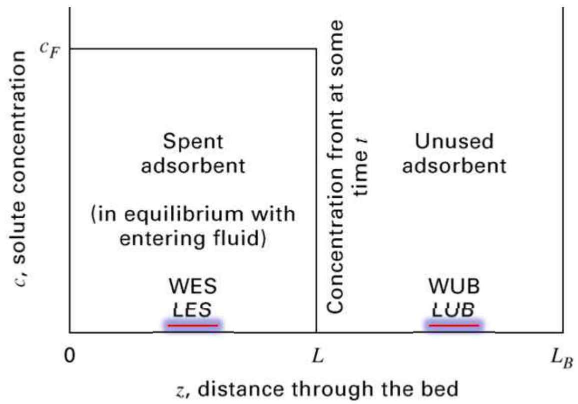
Lecture 6.
Kinetics and Transport in Sorption (3)

- Ideal Fixed-Bed Adsorption (Frontal Loading Mode)
- Solute Concentration Distributions in Frontal Loading
  - Mass-transfer zone (MTZ)
- Analytical Solution for Concentration
- Scale-Up Using Constant-Pattern Front

Ideal Fixed-Bed Adsorption (1)

- Assumptions in ideal (local-equilibrium) fixed bed adsorption (frontal loading mode)
  - Negligible external and internal transport-rate resistances
  - Ideal plug flow
  - Adsorption isotherm beginning at the origin





- The bed is divided into two zones or sections

  (1) Upstream of the stoichiometric front, $c_f = c_F$, spent adsorbent is saturated with adsorbate at a loading c_b^* in equilibrium with c_F

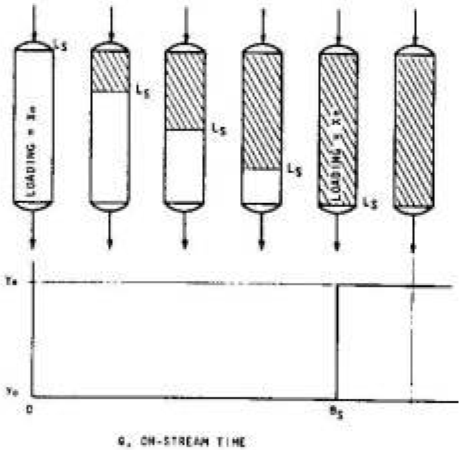
  (2) Downstream of the stoichiometric front, $c_f = 0$, the adsorbent is adsorbate-free

Ideal Fixed-Bed Adsorption (2)

- After a stoichiometric breakthrough time, t_s, the stoichiometric wave front reaches the end of the bed
  - $c_{f,out}$ abruptly rises to c_F
  - No further adsorption is possible

$$L_{\text{ideal}} \le L_B$$

L_B : length of packed bed
L_{ideal} : location of concentration wave front



Progress of ideal adsorption front

Effluent breakthrough curve

$$Q_F c_F t_{\text{ideal}} = \bar{c}_b^* A(1-\varepsilon_b)\rho_p L_{\text{ideal}}$$

c_b^* : loading in equilibrium with c_F

$$S = A(1-\varepsilon_b)\rho_p L_B$$

total mass of adsorbent in the bed

$$L_{\text{ideal}} = \text{LES} = \frac{Q_F c_F t_{\text{ideal}}}{\bar{c}_b^* S} L_B$$

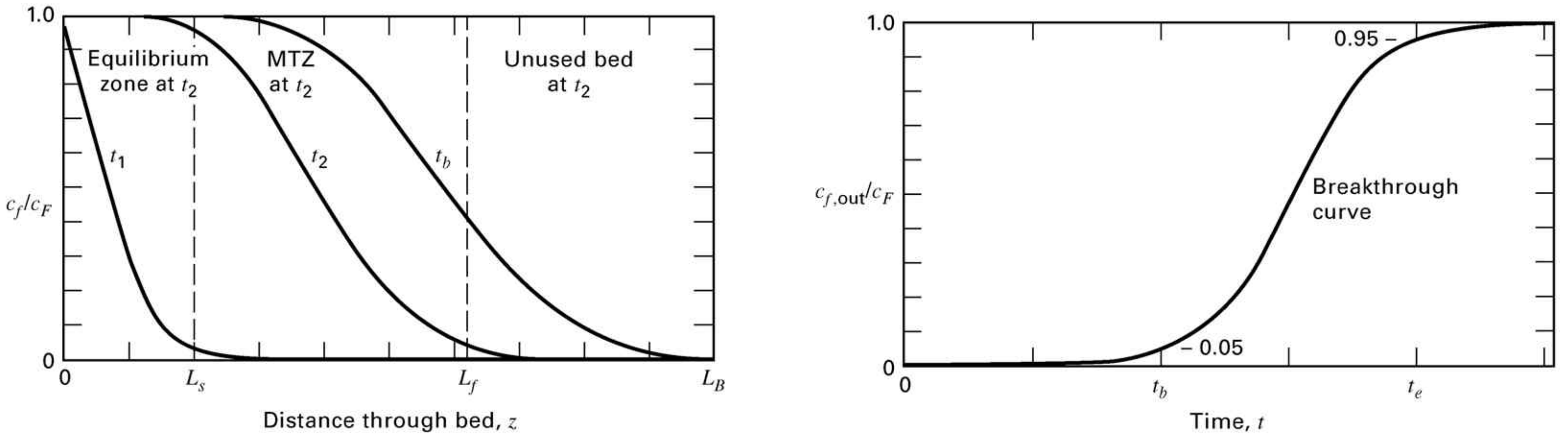
$$\text{LUB} = L_B - \text{LES}$$

$$\text{WES} = S\,\frac{\text{LES}}{L_B}$$

$$\text{WUB} = S - \text{WES}$$

Solute Concentration Distributions in Frontal Loading

- Actual solute concentration distributions of frontal are not ideal



  - At t_1, no part of the bed is saturated
  - At t_2, the bed is almost saturated for a distance L_s and almost clean at L_f; beyond L_f, little mass transfer occurs and the adsorbent is unused
    The region between L_s and L_f: mass-transfer zone (MTZ), where adsorption takes place
    L_f can be taken where $c_f/c_F = 0.05$, with L_s at $c_f/c_F = 0.95$
  - At t_b (breakthrough time), the leading point of the MTZ just reaches the end of the bed

Breakthrough concentration can be taken for $c_f/c_F = 0.05$ or minimum detectable (or maximum allowable) solute concentration in effluent fluid

Analytical Solution

- For an initially clean bed free of solute adsorbate (by Anzelius)

$$\frac{c_f}{c_F} \approx \frac{1}{2}\left[1+\operatorname{erf}\left(\sqrt{\tau}-\sqrt{\xi}+\frac{1}{8\sqrt{\tau}}+\frac{1}{8\sqrt{\xi}}\right)\right]$$

$$\xi = \frac{3k_{c,tot}z}{R_p u}\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)$$

Dimensionless distance coordinate

$$\tau = \frac{3\alpha k_{c,tot}}{R_p}\left(t-\frac{z}{u}\right)$$

Dimensionless displacement–corrected time coordinate

- Profiles of solute concentration in equilibrium with the average sorbent loading (by Klinkenberg)

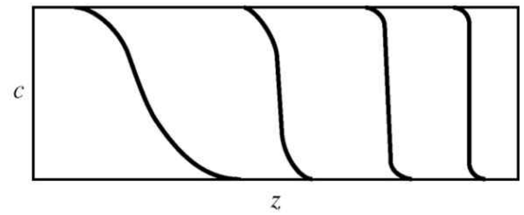
$$\frac{c_f^*}{c_F} = \frac{\bar{c}_b}{\bar{c}_b^*} \approx \frac{1}{2}\left[1+\operatorname{erf}\left(\sqrt{\tau}-\sqrt{\xi}-\frac{1}{8\sqrt{\tau}}-\frac{1}{8\sqrt{\xi}}\right)\right]$$

$c_f^* = \bar{c}_b\alpha$

$\bar{c}_b^*$ is the loading in equilibrium with c_F

Scale-Up Using Constant-Pattern Front (1)

- Persistent transport-rate resistance eventually limits self-sharpening, and an asymptotic or constant-pattern front (CPF) is developed
  - MTZ becomes constant
  - Curves of c_f / c_F and $\bar{c}_b / \bar{c}_b^*$ become coincident



- When the CPF assumption is valid, it can be used to determine the length of a full-scale adsorbent bed from breakthrough curves obtained in small-scale laboratory experiments

Total bed length

$$L_B = \mathrm{LES} + \mathrm{LUB}$$

Length of an ideal, equilibrium-adsorption section unaffected by mass-transfer resistance

$$\mathrm{LES} = \frac{Q_F c_F t_b}{q_F \rho_b A}$$

Scale-Up Using Constant-Pattern Front (2)

$$\mathbf{LUB} = \frac{L_e}{t_s}(t_s - t_b)$$

L_e/t_s : ideal wave-front velocity

- The stoichiometric time, t_s, divides the MTZ (e.g., CPF zone) into equal areas (t_s is equidistant between t_b and t_e)

$$t_s = \int_0^{t_e} \left(1 - \frac{c_f}{c_F}\right) dt$$

$$\mathbf{LUB} = \frac{\mathbf{MTZ}}{2}$$