

Adsorption Principles and Structure Characteristics of Porous Materials

(www.che.ncku.edu.tw/FacultyWeb/TengH) porous materials

Syllabus

1. Heterogeneous Reacting System – nonporous particles
2. Heterogeneous Reacting System – porous particles
“Chemical Reaction Engineering” Levenspiel, 2nd ed.
3. Physical Adsorption at the Gas-Solid Interface – Theory
“Principles of Colloid and Surface Chemistry” Hiemenz, 2nd ed
4. Powder Surface Area and Porosity - Technique
“Powder Surface Area and Porosity” Lowell and Shields, 3rd ed.
5. Crystal Structure
“Basic Solid State Chemistry” West, 2nd ed.

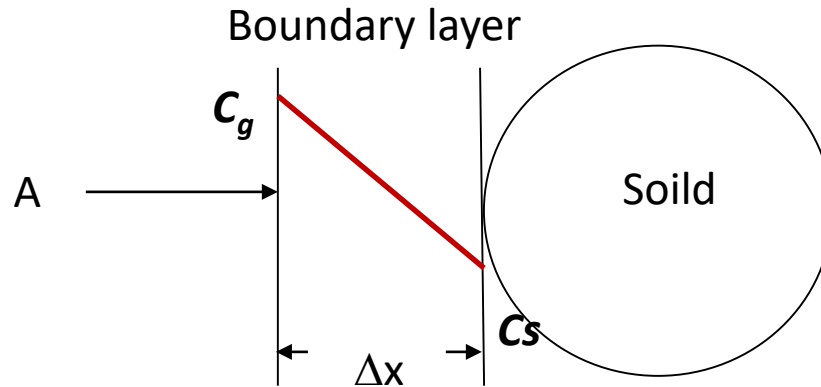
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Chapter 1

Heterogeneous Interacting System – Nonporous



concentration gradient

Reaction rate depends on mass transfer and chemical reaction on surface
(Interaction)

$$\begin{aligned}
 Q_{\text{transfer}} &= -\frac{1}{s} \frac{dN_A}{dt} \\
 \text{(Loss rate per unit area)} & \left. \begin{array}{l} \text{based on unit area of solid} \\ \text{not mass on volume} \end{array} \right\} \\
 Q_{\text{interaction}} &= -\frac{1}{s} \frac{dN_A}{dt} \\
 Q_g &= -\frac{1}{s} \frac{dN_A}{dt} = -D \frac{\Delta C}{\Delta x} = -\frac{D}{\Delta x} (C_s - C_g) \\
 &= -k_g (C_s - C_g) \text{ ----- (1)}
 \end{aligned}$$

where D is the diffusion coefficient and k_g is the mass transfer coefficient.

$$\frac{k_g d_p}{D} = 2 + 0.6 Sc^{\frac{1}{3}} Re^{\frac{1}{2}} = 2 + 0.6 \left(\frac{\mu}{\rho D} \right)^{\frac{1}{3}} \left(\frac{\rho u d_p}{\mu} \right)^{\frac{1}{2}}$$

Chemical reaction $Q_s = -\frac{1}{s} \frac{dN_A}{dt} = k_s C_s$ ----- (2)

At steady state : $Q_g = Q_s$

$$k_g (C_g - C_s) = k_s C_s$$

$$\underline{C_s} = \frac{k_g}{k_g + k_s} C_g$$

(conc. at the surface)

k_g depends on:

1. relative velocity
2. particle size
3. fluid properties

k_s depends on:

1. surface structure
2. No. of active sites

Substitute into (1) or (2)

$$-r_A = Q_g = Q_s = -\frac{1}{s} \frac{dN_A}{dt} = \frac{1}{\frac{1}{k_g} + \frac{1}{k_s}} C_g = k_{app.} C_g$$

If $k_g \gg k_s$ (transfer is fast)

$$-r_A = k_s C_g$$

If $k_s \gg k_g$ (mass transfer slow)

$$-r_A = k_g C_g$$

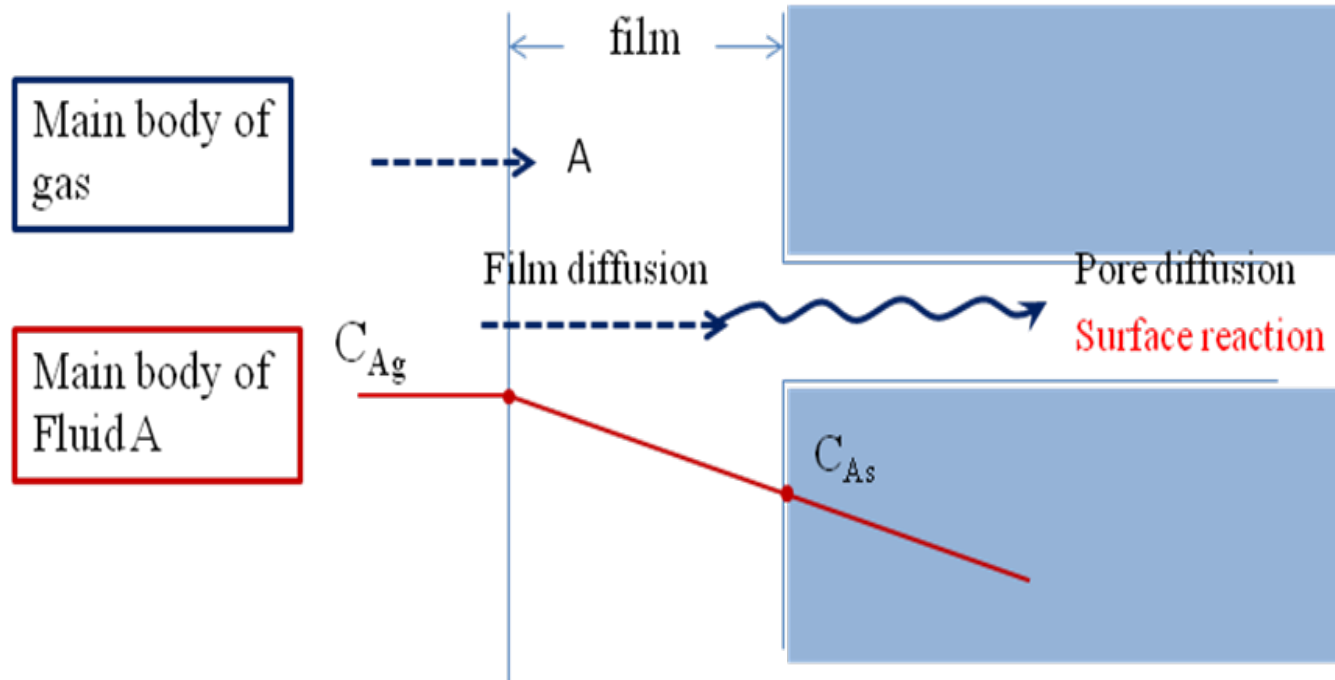
$$\therefore -r_A = \frac{k_s C_g}{1 + \frac{k_s}{k_g}}$$

where: is function of particle properties, defined as

Damkohler number (= $Da = \frac{\text{chemical reaction rate}}{\text{Interface diffusion rate}}$)

Chap. 2

Heterogeneous Interacting System – Porous Particles



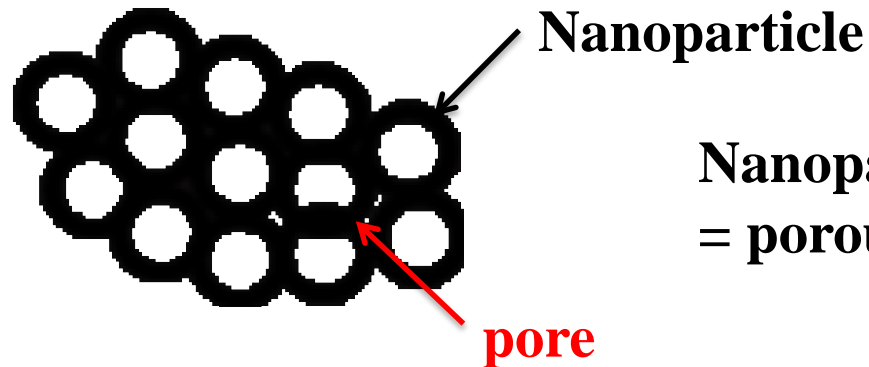
Surface area = internal + external
However internal SA \gg external SA

Reactions for a heterogeneous system

1. Gas film resistance
2. Pore diffusion resistance
3. Surface phenomenon resistance
(Adsorption, surface reaction, deposition)



Active site theory



All these pore structures have to be measured by the physical adsorption technique.