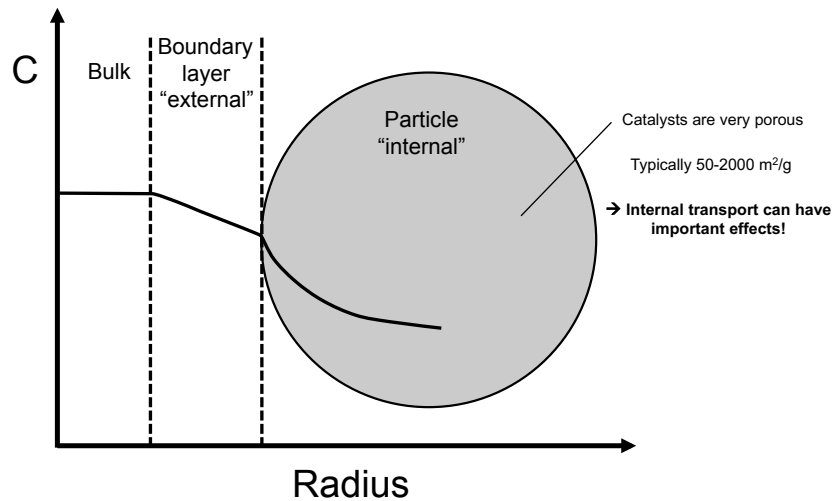


3 Transport effects in heterogeneous catalysis

Overview of the system:

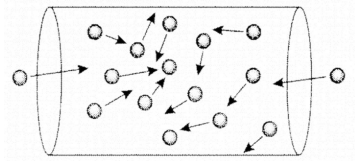


3

3 Transport effects in heterogeneous catalysis

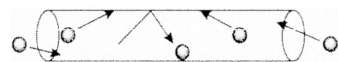
3.3.1 Types of pores and pore networks

- Molecular diffusion



In large pores (>1000 nm for molecules ~ 100 g/mol), molecules will hit themselves much more than the wall (=bulk diffusion)

- Knudsen diffusion



In smaller pores ($5 < R_p < 1000$ nm for molecules ~ 100 g/mol), molecules will increasingly hit the wall more than themselves

$$D_{KA} = 9.7 \cdot 10^3 R_{po} \left(\frac{T}{M_A} \right)^{1/2}$$

Knudsen diffusion coefficient [cm^2s^{-1}]

Pore radius [cm]

Molecular weight [g/mol]

T° [K]

For a gas, $D_{AB} \sim 0.1 \text{ cm}^2\text{s}^{-1}$. For D_{KA} to be comparable, for a molecule where $M_A \sim 100$ g/mol and $T^\circ = 300$ K, we need:

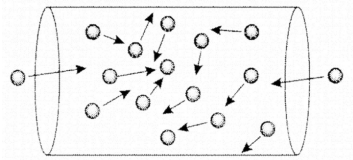
$$0.1 = 10^4 R_{po} (3)^{1/2} \rightarrow R_{po} \sim 10^{-5} \text{ cm} = 100 \text{ nm}$$

4

3 Transport effects in heterogeneous catalysis

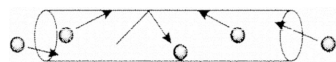
3.3.1 Types of pores and pore networks

- Molecular diffusion



In large pores (>1000 nm for molecules ~ 100 g/mol), molecules will hit themselves much more than the wall (=bulk diffusion)

- Knudsen diffusion



In smaller pores ($5 < R_p < 1000$ nm for molecules ~ 100 g/mol), molecules will increasingly hit the wall more than themselves

- Single file diffusion



Only one molecule can pass through the pore at a time (2-5 nm, depending on the molecule)

- Shape-selective/very small pore



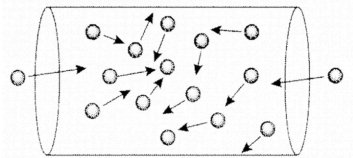
The pore is smaller than a molecule (< 2 nm)

5

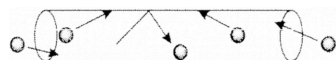
3 Transport effects in heterogeneous catalysis

3.3.1 Types of pores and pore networks

- Molecular diffusion



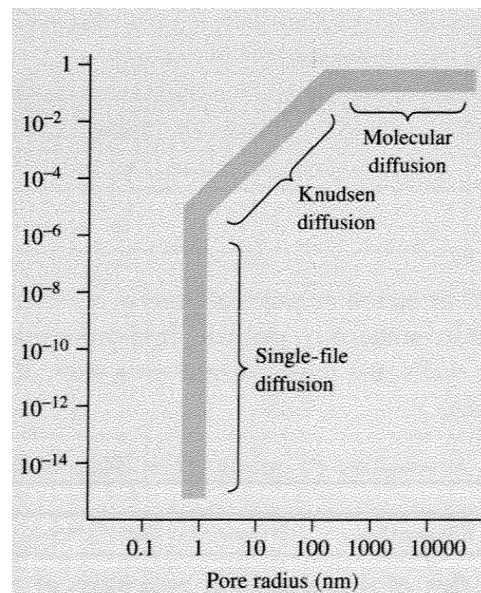
- Knudsen diffusion



- Single file diffusion



- Shape-selective/very small pore



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