Research Summary

Molecular Modeling of Filtration in Nanoporous Media

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Objectives

- Explain the concept of selective permeability
- Predict the movement of the molecules across the membrane based on their composition
- Interpret and graph kinetics of molecule transport across the semi-permeable membrane

Semi-permeable membrane allows

- Only small molecules to cross.
- Only charged molecules to cross.
- Certain molecules to enter the membrane but not cross to the other side.
- Molecules to cross the membrane until they reach equal concentration on both sides.
- Molecules to cross dependent upon their chemical characteristics.

Diffusion

"The movement of particles in a solid from an area of **high** concentration to an area of **low** concentration resulting in the uniform distribution of the substance"

- During diffusion molecules move down a concentration gradient

$$J = -D\frac{dC}{dx}$$

D- diffusion coefficient

Diffusion Coefficient

- Diffusion coefficient increases with increasing temperature (T)

$$D = \rho_g d_p \left(\frac{8RT}{\pi M}\right)^{\frac{1}{2}} e^{-\frac{\Delta E}{RT}}$$

D = diffusion coefficient [m^2/s]

D_o = pre-exponential [m^2/s]

Q_d = activation energy [J/mol or eV/atom]

R = gas constant [8.314 J/mol-K]

T = absolute temperature [K]

Permeability coefficient

$$P = D_{c,ads} * \left(\frac{d\ln(p)}{d\ln(C_{ads})}\right)\left(\frac{\theta}{\tau}\right)\frac{dC_{ads}}{dp} + \frac{\theta}{\tau}\frac{D_{c,gas}}{RT}$$

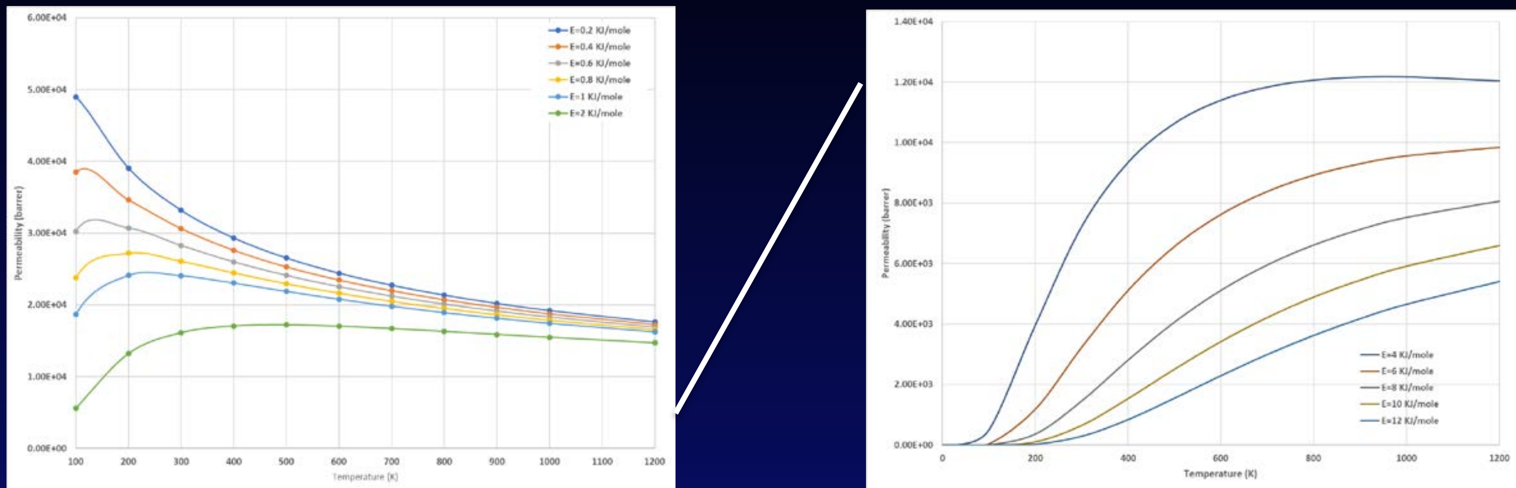
$$D_{c,ads} = \rho_g d_p \left(\frac{8RT}{\pi M}\right)^{\frac{1}{2}} e^{\frac{-E_{ads}}{RT}}$$

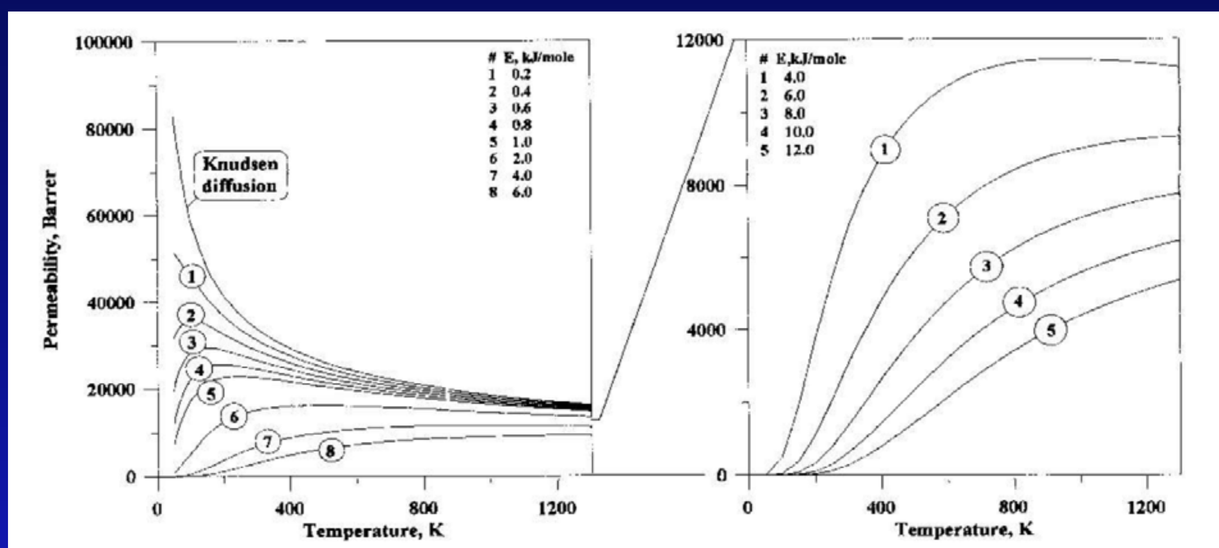
$$D_{c,gas} = \rho_g d_p \left(\frac{8RT}{\pi M}\right)^{\frac{1}{2}} e^{\frac{-E_{gas}}{RT}}$$

For permanent gases:

$$P = \rho_g d_p \left(\frac{8}{\pi RTM}\right)^{\frac{1}{2}} \frac{\theta}{\tau} e^{\frac{-E_{gas}}{RT}}$$

Upper bound of permeability coefficient





Shelekhin et al., 1995

Selectivity of gas separation

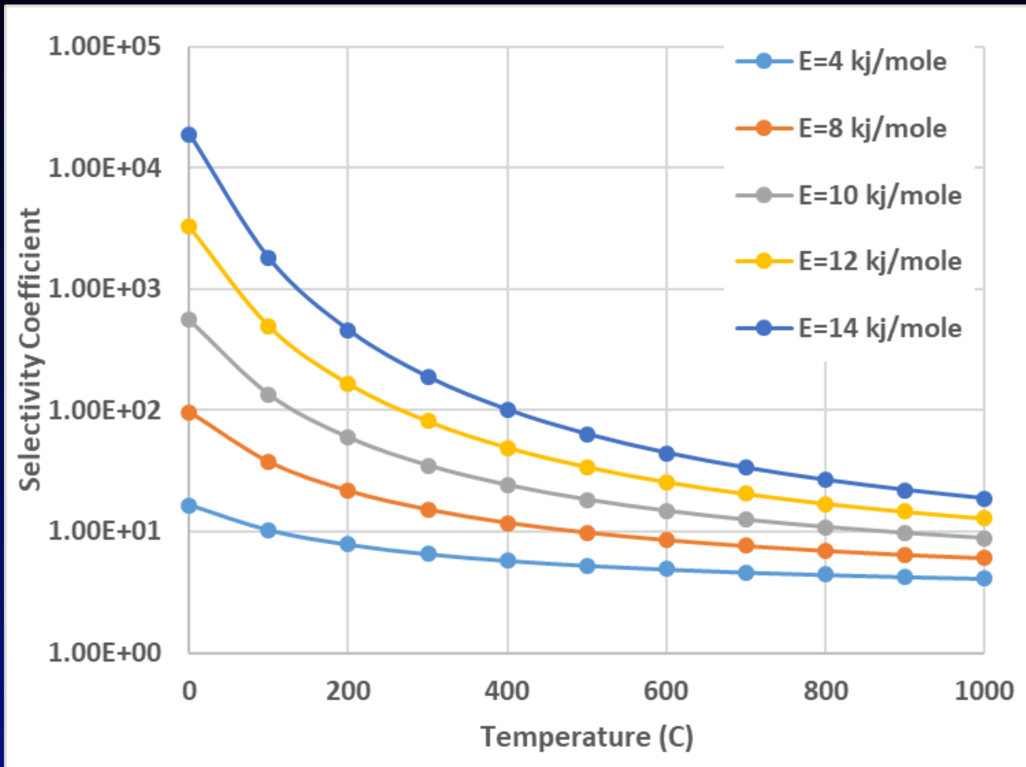
- Selectivity factor is defined as the ratio of the permeability coefficients

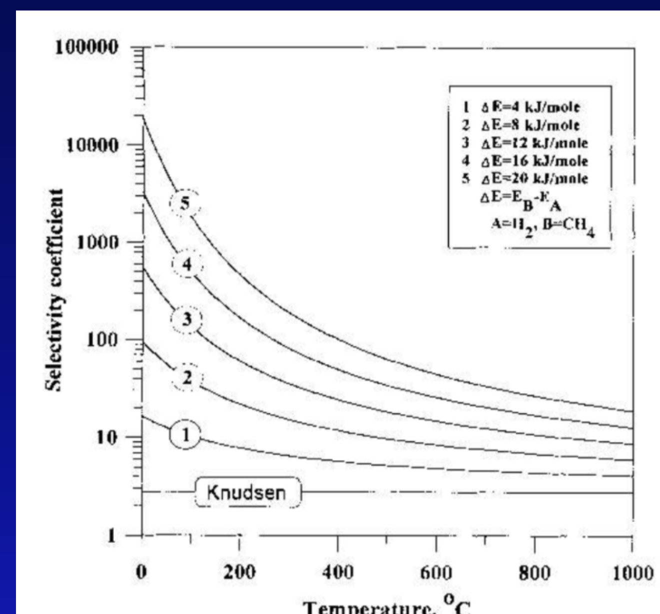
- Only exponential term depends on temperature

$$\alpha = \frac{P_a}{P_b} = \left(\frac{M_B}{M_A}\right)^{\frac{1}{2}} \exp\left(-\frac{\Delta E_A - \Delta E_B}{RT}\right)$$

Shelekhin et al., 1995

Selectivity of gas separation





Shelekhin et al., 1995

Future Works

- Determine the dependence of permeability coefficients on temperature
- Determine the dependency of activation energy of diffusion and pore size kinetic diameter
- Create a theoretical model of gas permeation in microporous molecular-sieve membranes

Shelekhin et al., 1995

Thank you!
Question?