How to determine empirical factors

1. k_f (gas film mass transfer coefficient)

- based on diluted packed bet experimental

Sh : $Sh = 1.42 + 0.92\,Sc^{1/3}Re^{0.6}$

2. D_{eff} (effective diffusion coefficient)

- based on Knudsen and molecular diffusion
- approximated by Modified Bruggeman[1]

$$D_{eff}: \quad D_{eff} = \varepsilon^{\alpha} D_{pore}, \qquad \frac{1}{D_{pore}} = \frac{1}{D_{CO_2,N_2}} + \frac{1}{D_{kn}}$$

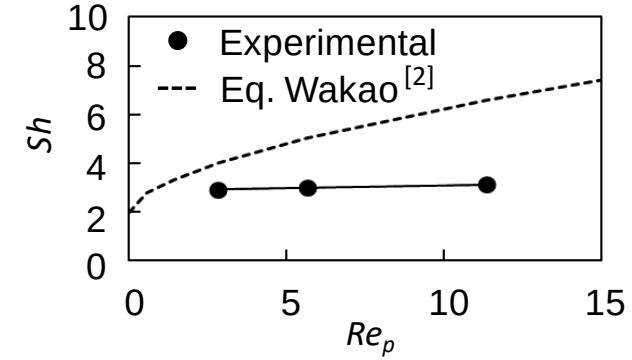
constant

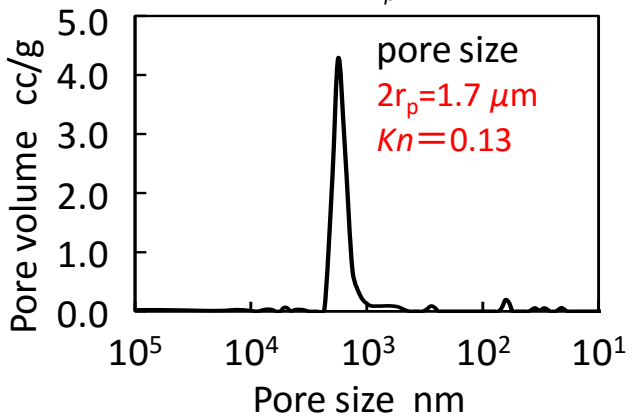
$$D_{Kn} = \frac{4}{3} r_p \sqrt{\frac{2RT}{\pi M_{CO_2}}} \qquad D_{CO_2,N_2} = \frac{0.00266\,T^{3/2}}{P M_{CO_2,N_2}^{1/2} \sigma_{CO_2,N_2}^{2} \Omega_D}$$

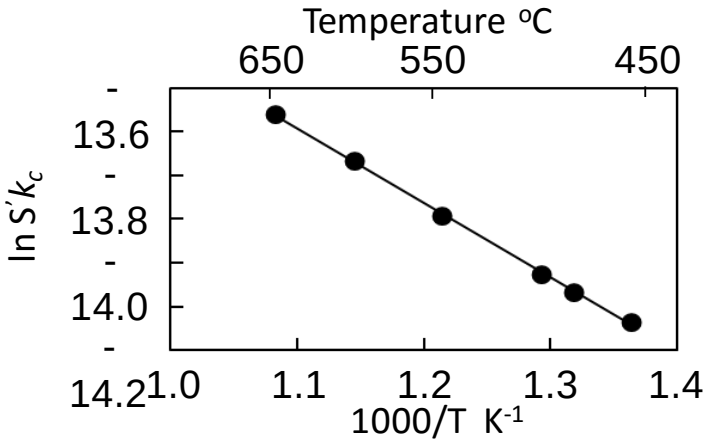
3. k_c (surface chemical reaction coefficient)

- based on experimental data of 100% CO_2 conditions

$$k_c: \quad k_c = 1.16 \times 10^{-1} \exp\left(-\frac{1.42 \times 10^4}{RT}\right)$$







[1] D.A.G. Bruggeman ;Ann. Physik. 24 636 1935

[2] N. Wakao and T. Funazkri : chem Eng. sci 33 1375(1978)