

Hindered solute transport

Hydrodynamic coefficients $K_{i,d}$ and $K_{i,c}$ introduced in eq 1 account for the effect of the finite pore size on diffusion and convection through pores. Several approximate relations of these hydrodynamic factors are available in the literature.⁴⁵ Analytical relations derived by Bungay and Brenner are among the most interesting ones as they were established for the entire range of solute to pore size ratios⁴⁵

$$K_{i,d} = \frac{6\pi}{K_{i,t}} \quad (\text{I})$$

$$K_{i,c} = \frac{(2 - (1 - \lambda_i)^2)K_{i,s}}{2K_{i,t}} \quad (\text{II})$$

where $K_{i,t}$ and $K_{i,s}$ are defined as

$$K_{i,t} = \frac{9}{4}\pi^2\sqrt{2}(1 - \lambda_i)^{-5/2} \left[1 + \sum_{n=1}^2 a_n (1 - \lambda_i)^n \right] + \sum_{n=0}^4 a_{n+3} \lambda_i^n \quad (\text{III})$$

$$K_{i,s} = \frac{9}{4}\pi^2\sqrt{2}(1 - \lambda_i)^{-5/2} \left[1 + \sum_{n=1}^2 b_n (1 - \lambda_i)^n \right] + \sum_{n=0}^4 b_{n+3} \lambda_i^n \quad (\text{IV})$$

with $a_1 = -73/60$, $a_2 = 77.293/50.400$, $a_3 = -22.5083$, $a_4 = -5.6117$, $a_5 = -0.3363$, $a_6 = -1.216$, $a_7 = 1.647$, $b_1 = 7/60$, $b_2 = -2.227/50.400$, $b_3 = 4.0180$, $b_4 = -3.9788$, $b_5 = -1.9215$, $b_6 = 4.392$, $b_7 = 5.006$ and $\lambda_i = r_{i,Stokes} / r_p$ where is $r_{i,Stokes}$ stands for the Stokes radius of the ion i defined as follows

$$r_{i,Stokes} = \frac{k_B T}{6\pi\eta D_i} \quad (\text{V})$$

where k_B is the Boltzmann constant and η is the solution viscosity.