Supporting Information

Unique selectivity trends of highly permeable PAP[5] water channel membranes

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Debye length (λ_D) calculation

The Debye length (λ_D, nm) of various ionic solutions is calculated by the equation,

$$\lambda_D = \sqrt{\frac{\varepsilon_0 \varepsilon_r k_B T}{2 N_A e^2 I}} \quad (1)$$

where ε_0 and ε_r are vacuum and relative permittivity, k_B is the Boltzmann constant, T is the absolute temperature (K), N_A is the Avogadro's number, e is the elementary charge and I is the ionic strength (mol·L^{-1}) of the solution.[1] The ionic strength of the solution is defined as

$$I = {}^{1}/_{2} \Sigma c_i z_i^{\,2} \quad (2)$$

where c_i and z_i are molar concentration (M) and valence number of charged ions, respectively.[2] For the methyl blue dye rejection test, the ionic strength of the solutions was adjusted using NaCl.

Donnan rejection calculation

Theoretical Donnan rejections for various ionic solutes in **Figure 3A** were calculated by following equation.[3]

$$R = 1 - \left(\frac{|z_i| c_i}{|z_i| c_i^{\,m} + c_x^{\,m}} \right)^{|z_i / z_j|} \quad (3)$$

where c_i and $c_i^{\,m}$ are co-ion (same charge ions with membrane) concentrations of feed solution and membrane, $c_x^{\,m}$ is the charge concentration of the membrane, i and j represents the opposite charge signs, and z is the ionic valence number. $c_i^{\,m}$ is generally adapted as the co-ion concentration of the permeate solution.[3] $c_x^{\,m}$ is obtained by fitting the experimental rejection value of $Ru(bipy)_3Cl_2$ (91.56 %) into equation (3), as shown in following equation.

$$c_x^{\,m} = \frac{|z_i| c_i}{(1-R)^{|z_j / z_i|}} - |z_i| c_i^{\,m} = \frac{|z_i| c_i}{(1-R)^{|z_j / z_i|}} - |z_i| \left(c_i \times (1-R) \right) = \\ = 3.5 mM$$

Critical flux (J_c) calculation

The critical flux of the ML-PAP[5] membrane is calculated by the equation,[4-6]

$$J_c = \frac{\varepsilon k_B T}{\eta R_p^{\,2}} \quad (4)$$

where ε is the porosity of the ML-PAP[5] membrane, η is the viscosity of the solution and R_p is the pore radius of the membrane. For the ML-PAP[5] membrane, within a $1\ \mu m \times 1\ \mu m$ unit area, the actual channel number is $\sim 4.2 \times 10^5$ and the pore radius was adapted from the radius of confined pillar[5]arene of the PAP[5] channels (0.25 nm).[7] Therefore, the ε is calculated as

$$\varepsilon = \frac{4.2 \times 10^5 \times \pi r^2}{1\ \mu m \times 1\ \mu m} = 0.0824$$

and the J_c is calculated as

$$J_c = \frac{0.0824 \times 1.38 \times 10^{-23} m^2 kg s^{-2} K^{-1} \times 293K}{(0.25 \times 10^{-9} nm)^2 \times 0.001 kg m^{-1} s^{-1}} \times \frac{mol\ H_2O}{0.000018\ m^3} = 296{,}000\ {}^{mol}/_{m^2 s}$$

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