

Supplementary Material.

From Ion Current to Electroosmotic Flow Rectification in Asymmetric Nanopore Membranes

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Calculations of Percent of Ions in the Double Layer and Transference Number

To simplify our calculations, we assume that the tip is a cylinder of length h and radius r . The tip walls have a surface charge density of -12 mC m^{-2} , based on previously reported values for polyethylene terephthalate (PET) [1,2]. Inside the tip, there is a solution of 10 mM KCl which gives a thickness of the electrical double layer (Debye length) of 3 nm at 25 °C.

The surface charge density on the pore tip walls can be converted to a number of moles of carboxylate groups at the surface of the cylinder, n_{COO} , according to Equation S1, where F is the Faraday constant.

$$n_{COO} = \frac{1.2 \times 10^{-6} \times 2\pi r h}{F} \quad \text{Equation S1}$$

If we assume an equivalent number of moles of cations (K^+) in the electrical double layer, n_{dl} (Equation S2).

$$n_{dl} = n_{COO} = \frac{1.2 \times 10^{-6} \times 2\pi r h}{F} \quad \text{Equation S2}$$

To a first approximation, the number of moles of ions, n_b , which is the sum of the numbers of moles of K^+ and Cl^- , $n_{K,b}$ and $n_{Cl,b}$ respectively, in the bulk solution in the pore tip is determined by the bulk concentration (10 mM) (Equation S3).

$$n_b = n_{K,b} + n_{Cl,b} = 2 \times 10^{-5} \times \pi (r - 3 \times 10^{-7})^2 h \quad \text{Equation S3}$$

Therefore the fraction of total number of moles of ions that are double layer cations, as a function of r , the radius of the pore tip in nm, is

$$\%_{dl} = \frac{n_{dl}}{n_b + d_{dl}} = \frac{0.12 r}{0.12 r + F \times 10^{-7} (r-3)^2} \times 100 \quad \text{Equation S4}$$

The transference number of cations (K^+) through the tip, t_+ , is defined as [3]

$$t_+ = \frac{(n_{dl} + n_{K,b}) \times u_{Na}}{(n_{dl} + n_{K,b}) \times u_K + n_{Cl,b} \times u_{Cl}} \quad \text{Equation S5}$$

Where u_K and u_{Cl} are the mobilities of K^+ and Cl^- , respectively.

Considering $u_K = 7.619 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1} \text{ V}^{-1}$ and $u_{Cl} = 7.912 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1} \text{ V}^{-1}$ [3],

$$t_+ = \frac{(0.24 r + F \times 10^{-7} (r-3)^2) \times 7.619}{1.8286 r + 15.824 F \times 10^{-7} (r-3)^2} \quad \text{Equation S6}$$

References

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