Supplementary Information

Influence of temperature gradients on charge transport in asymmetric nanochannels

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S1. Temperature dependence of physical properties

Permittivity data was obtained from.¹ The diffusion coefficients are based on molar conductivity data of Benson and Gordon² and converted to diffusion coefficients by \( D_i = (RTA)/(z^2F^2) \). Viscosity and thermal conductivity were obtained from the NIST Chemistry Webbook.³ All values are 1 at \( T_0 \) of 293 K and increase or decrease with \( \theta \), dimensionless temperature \((T - T_0)/T_0\).

\[
\epsilon_r = 1 - 1.2984\theta
\]
\[
D_1 = 1 + 8.4585\theta
\]
\[
D_2 = 1 + 8.8466\theta
\]
\[
\mu = \exp(-6.46\theta)
\]
\[
k = 1 + 0.8098\theta
\]
S2. Boundary conditions for simulations

The boundary conditions below are used for the corresponding boundaries as shown in Figure 1 of the manuscript, which are identical to the boundary conditions previously used.\textsuperscript{4,5}

**AB**

Dirichlet/Constant value for $\varphi$, $\theta$ and $c_i$

$\varphi = \frac{V_0}{V_{\text{ref}}} \text{ or } 0$

$\theta = \theta_{\text{left}}$

$c_i = 1$

Zero flux for $\psi$

$n \cdot (\epsilon_r \nabla \psi) = 0$

Open Boundary for Velocity

$[-pI + \mu \nabla \bar{u}]n = 0$

**BC and FG**

Symmetry/No normal velocity component

Insulating/Zero Flux for $\theta$, $c_i$, $\varphi$ and $\psi$

**CD and EF**

No-slip for velocity ($\bar{u} = 0$)

Insulating/Zero Flux for $\theta$ and $c_i$

**DE**

$\psi = \frac{V_{\text{wall}}}{V_{\text{ref}}}$

No-slip for velocity ($\bar{u} = 0$)

Insulating/Zero Flux for $\theta$, $c_i$ and $\varphi$

**GH**
Dirichlet/Constant value for ϕ, θ and $c_i$

$\varphi = V_0/V_{\text{ref}}$ or 0

$\theta = \theta_{\text{right}}$

$c_i = 1$

Zero flux for $\psi$

$n \cdot (\epsilon_r \nabla \psi) = 0$

Open Boundary for Velocity

$[-pI + \mu \nabla \bar{u}]n = 0$

AH

Symmetry conditions

References

(1) Kaatze, U. Complex permittivity of water as a function of frequency and temperature.  

(2) Benson, G. C.; Gordon, A. R. A reinvestigation of the conductance of aqueous solutions
 of potassium chloride, sodium chloride, and potassium bromide at Temperatures from

(3) Lemmon, E.; McLinden, M.; Friend, D. Thermophysical Properties of Fluid Systems.  
http://webbook.nist.gov/, In NIST Chemistry WebBook, NIST Standard Reference
 Database Number 69, Eds. P.J. Linstrom and W.G. Mallard, National Institute of Stan-

(4) Wood, J. A.; Benneker, A. M.; Lammertink, R. G. Temperature effects on the elec-