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 Gordon[2] and converted to diffusion coefficients by $D_i = (RT\Lambda)/(z^2F^2)$. 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 θ, dimensionless temperature $(T - T_0)/T_0$.

$$\epsilon_r = 1 - 1.29840\theta$$

$$D_1 = 1 + 8.45850\theta$$

$$D_2 = 1 + 8.84660\theta$$

$$\mu = \exp(-6.460\theta)$$

$$k = 1 + 0.80980\theta$$

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.[4,5]

AB

Dirichlet/Constant value for φ, θ and c_i

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

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

$c_i = 1$

Zero flux for ψ

$\mathbf{n} \cdot (\epsilon_r \nabla \psi) = 0$

Open Boundary for Velocity

$[-p\mathbf{I} + \mu \nabla \bar{u}]\mathbf{n} = 0$

BC and **FG**

Symmetry/No normal velocity component

Insulating/Zero Flux for θ, c_i, φ and ψ

CD and **EF**

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

Insulating/Zero Flux for θ and c_i

DE

$\psi = V_{\mathrm{wall}}/V_{\mathrm{ref}}$

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

Insulating/Zero Flux for θ, c_i and φ

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 ψ

$\mathbf{n} \cdot (\epsilon_r \nabla \psi) = 0$

Open Boundary for Velocity

$[-p\mathbf{I} + \mu \nabla \bar{u}]\mathbf{n} = 0$

AH

Symmetry conditions

References

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