Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Tripling the Reverse Electrodialysis Power Generation in Conical Nanochannels Utilizing Soft Surfaces

Mahdi Khatibi [a], Arman Sadeghi [b], Seyed Nezameddin Ashrafizadeh [a,*]

[a] *Research Lab for Advanced Separation Processes, Department of Chemical Engineering, Iran University of Science and Technology, Narmak, Tehran 16846-13114, Iran*

[b] *Department of Mechanical Engineering, University of Kurdistan, Sanandaj 66177-15175, Iran*

The present model performance was validated by comparing the model predictions with the experimental data of Laucirica et al.[1]. In the work conducted by Laucirica et al., a bullet-shaped nanochannel was fabricated via track etching method in a polyethylene terephthalate (PET) foil of 12 μm thickness. The base radius (R_B) of the nanochannel was approximately 95 nm and the surface of the nanochannel was cation selective. To compare the model outputs with the experimental data of Laucirica et al.[1], it was assumed that the diffusion of ions occurs from the base-end reservoir towards the tip-end reservoir ($C_H > C_L$). Moreover, the geometric parameters of the nanochannel system were considered as: $R_T = 10$ nm, $L_R = R_R = 200$ nm, $L_N = 1200$ nm, $R_B = 95$ nm, $R_S = 5$ nm, and $C_H/C_L = 1000$. In addition, the volumetric PEL fixed charge density was considered to be $\mathbb{N}_{PEL}/N_A = 126$ molm^{-3}, the value which is equal to the charge density of a pH-responsive rigid nanochannel at pH = 10. It should be noted that the nanochannel used in the experimental work is solid-state, so the value chosen for the soft layer charge density was equivalent to the surface charge density of the solid-state nanochannel. Fig. S1

* Corresponding author: ashrafi@iust.ac.ir (S.N. Ashrafizadeh)
Co-authors: m_khatibi@chemeng.iust.ac.ir (M. Khatibi); a.sadeghi@eng.uok.ac.ir (A. Sadeghi)

compares the power output predicted by the present theoretical model with the experimental data of Laucirica et al.[1]. As demonstrated in Fig. S1, our model successfully reproduces the experimental data of Laucirica et al.[1]. This indicates that the present model provides close-to-reality predictions, and the conclusions made in the current study, including the maximum power generation improvement by covering the nanochannel inner surface with PELs, is practically achievable.

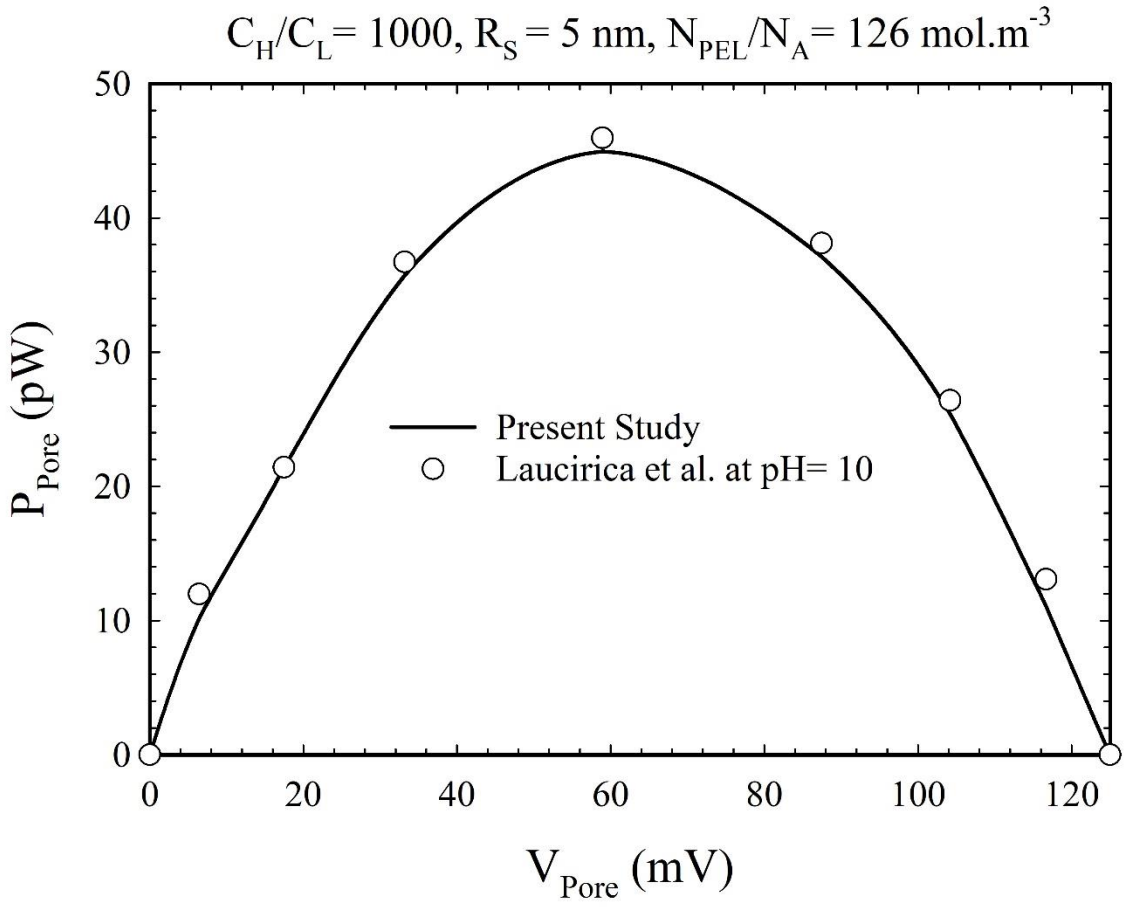

Fig. S1. Comparison of the voltage-power results predicted by the present model and the experimental data of Laucirica et al.[1].

References

1. G. Laucirica, A. G. Albesa, M. E. Toimil-Molares, C. Trautmann, W. A. Marmisollé and O. Azzaroni, *Nano Energy*, 2020, **71**, 104612.