Study of ionic transport spatially varying ion diffusivity in capacitive deionization

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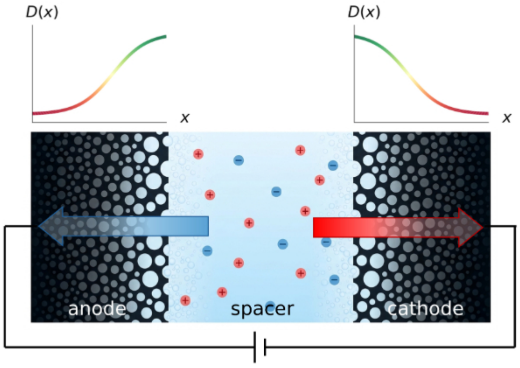
Capacitive deionization (CDI) is an emerging technology for water desalination based on ion electrosorption in porous carbon electrodes [1]. Classical continuum models for capacitive deionization (CDI) typically assume a uniform ion diffusion coefficient across the entire cell, despite the strong heterogeneity of porous electrodes. However, experimental observations and pore-scale considerations suggest that ion transport inside the electrode is hindered by structural factors such as tortuosity, water affinity and pore accessibility [2], which are not explicitly captured in standard models.
In this work, we extend a previously developed one-dimensional CDI model [3] by introducing a spatially dependent effective diffusion coefficient to account for transport limitations within porous electrodes. Several physically motivated profiles are explored, representing reduced ion mobility toward the inner regions of the electrode. The modified model is solved numerically and compared against the baseline constant-diffusion formulation.
Results show that spatial variations in diffusivity significantly affect the transient dynamics of ion transport, leading to slower ion depletion in the inner electrode regions while preserving equilibrium adsorption levels. This behavior is consistent with the separation of time scales between electromigration and diffusion previously reported. The proposed approach provides a simple yet effective way to incorporate electrode microstructure effects into continuum CDI models without increasing their complexity.
These findings highlight the importance of accounting for spatial transport limitations when interpreting experimental data and optimizing electrode design in CDI systems.

Keywords:
capacitive deionization (CDI), porous electrodes, spatially dependent diffusion, ion transport



Schematic of a CDI cell with depth-dependent transport. Top plots show a representative diffusion coefficient profile D(x), reflecting hindered diffusion due to a possible pore size distribution. Fading arrows indicate resistance as ions penetrate the electrode bulk.

References:

[1] Datar, S. D. et al., *Water Environ. Res.* 94(3), e10696 (2022).
[2] Liu, M. et al. , *Desalination* , 526, 115520 (2022).
[3] Lirio Piñar, J. A. et al. , *Phys. Rev. E* , 110, 034610 (2024).

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