Relaxed Adsorption-flow Coupling Enables Stable COMSOL Multiphysics® Modeling Of Upscaled Capacitive Deionization

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Abstract

The rapidly increasing world population will dramatically expand the future global freshwater requirements, now making lots of researchers realize the fundamental importance of developing effective desalination technologies. Hence, the emerging capacitive deionization (CDI) desalination technique is increasingly grabbing the attention of researchers. Simulation of capacitive desalination brings critical value for the understanding, prediction, and optimization of the CDI process which works on the principles of charging and discharging supercapacitors. Typically, a CDI cell comprises two porous electrodes separated by a nonconducting spacer, wherein it produces freshwater by allowing an applied voltage to rapidly extract the salt ions from the steadily passing water steam (during charging of the supercapacitor). Similarly, the electrodes are regenerated by discharging the adsorbed ions into a waste stream. Previous modeling attempts use the seminal state-of-the-art 2D-FEM method which simulates ion transport coupled with an electric-double-layer (EDL) adsorption formulation. There, the COMSOL Multiphysics® PDE interface implements large systems of interconnected adsorption-flow PDEs, and the resulting model was usually found to be "unsteady". In contrast, in the present work, we reinterpret the phenomena from a porous-catalyst perspective, which fundamentally breaks through the complexity wall by naturally relaxing the adsorption-flow coupling. Specifically, the Brinkman Equations simulated generalized water-flow patterns, which became the background flow in a Multiphysics-coupled Transport of Diluted Species in Porous Media. The latter thus effectively simulates both ionic transport and, through the Reactions interface, the time-dependent ion adsorption. Here, an accurate 0D Randles-circuit model pre-calculates the reaction rate to reduce simulation complexity. This approach reduces the detailed resolution but retains the ability to identify localized phenomena such as concentration shocks, and reaches the state-of-the-art performance in simulating global experimental metrics, as validated with literature data. Additionally, the decoupled Brinkman-flow calculations enable broad flow simulations and simulating the flow efficiency in complex and upscaled CDI structures. Ultimately, the approach means the new model greatly improves stability and broadly opens up research to large interconnected modules and nonlinear flow patterns. As the CDI field continues to grow, these large-scale systems will become increasingly important modeling targets, and we fundamentally believe this work will facilitate and promote future COMSOL Multiphysics® studies in modular CDI design.

Figures used in the abstract

Figure 1 : The image shows the time-dependent salt-ion concentration when two parallelly stacked capacitive deionization (CDI) cells operate to desalinate water. Here, COMSOL Multiphysics® straightforwardly simulates upscaled and structurally complex CDI modules by