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Salt rejection in flow-between capacitive deionization devices

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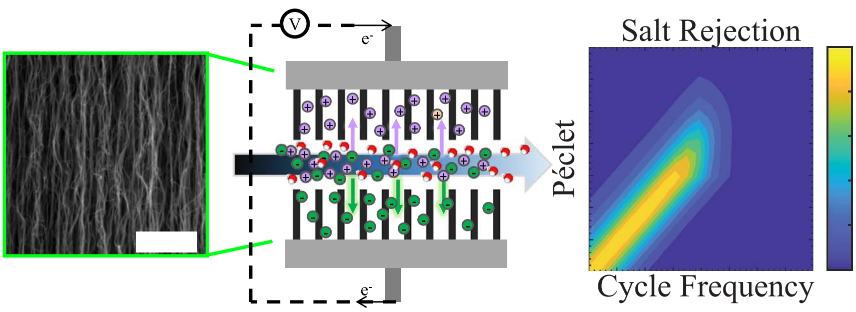
GRAPHICAL ABSTRACT



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ABSTRACT

Desalination technologies can increase potable water supplies worldwide. One possible approach, capacitive deionization (CDI), could prove optimal for brackish water treatment. At present, CDI development has largely focused on increasing salt adsorption capacity and desalination rates of materials and devices. In addition to these metrics, ultimately, optimizing salt rejection and throughput will be essential. In this work, we present a framework for the design of flow-between CDI cells for maximum salt rejection. We developed a model that is dependent on device specific parameters (system volume, flow rate, inlet and outlet water quality), to generalize the design of a cell for any given requirement. We showed that decreasing the advection-diffusion Péclet number and increasing the aspect ratio of the electrode compared to the channel space yield the highest salt rejection. In addition, tuning the cycle frequency time for salt rejection instead of complete electrode charging can yield faster water production rates and optimal salt rejection. These modeling results were validated through experimental prototypes that made use of vertically-aligned carbon nanotube (VA-CNT) electrodes. This framework to maximize salt rejection can be extended to a multitude of porous electrodes used in flow-between CDI devices.

1. Introduction

Less than 1% of the world's 1.4 billion km^3 of water is available freshwater. 98% of the world's water is in the form of brackish and seawater (1000–35,000 ppm or 10–600 mM NaCl concentration) [1]. Desalination can increase our water supplies, generating sufficient resources for household, industrial, and agricultural uses as well as mitigate the escalating water crisis [2]. One approach for desalination is

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Nomenclature			
δ	boundary layer thickness	F	Faraday's constant
ϵ	electrode porosity	f	electrode voltage cycling frequency
η	charge efficiency	h_p	inverse electrode surface area to volume ratio
κ	solution conductivity	I	current
$\bar{c}_{out}$	average effluent concentration	$j_{v,salt}$	salt flux to the electrode surface
Φ	flow rate	L_c	flow cell channel length
τ	electrode charging time constant	L_e	electrode thickness
l_t	electrode tortuosity	L_{rat}	ratio of electrode to spacer thickness
$\widetilde{Pe}$	modified Péclet number	L_{sp}	flow cell half spacer width
A_o	constant to satisfy the exponential function	N	salt flux
b	flow cell width	Q	electrode charge
c	concentration in the spacer	S_{ads}	salt adsoption
c_∞	bulk concentration	S_{rate}	salt adsorption rate
c_e	concentration in the electrode	SR	salt rejection
c_{rem}	electrode maximum concentration of salt adsorbed	T	temperature
D_e	electrode effective diffusivity	t	time
D_{NaCl}	sodium chloride diffusivity	x	spatial coordinate in the direction of flow
		y	spatial coordinate perpendicular to the flow
		SAC	salt adsorption capacity

capacitive deionization (CDI) (Fig. 1a), where a voltage is applied across high surface area electrodes and salt water flows between, driving charged ions in solution (such as sodium and chloride, but also heavy metals and other charged molecules) to adsorb at the electrode surface within the electric double layer (EDL), yielding desalinated effluent [3-5]. In order to maximize the desalination throughput and realize the potential of CDI, research has focused on increasing salt adsorption capacity (SAC) of high surface area materials and developing modeling tools to understand the physics and performance of devices [6].

Previously, many carbon materials with surface areas from a few hundred to a few thousand m^2/g have been studied for CDI [7, 8], leading to hierarchical materials with SAC of ~ 25 mg/g [9]. In addition to designing CDI prototypes for high salt adsorption, other metrics to consider have been capacitance, charge efficiency, and salt adsorption rate (SAR) [6, 10, 11]. However, the SAR metric does not provide a complete understanding of desalination performance. It is not only dependent on the electrode material properties (surface area, tortuosity, porosity, electrode thickness), but also on the device design and operational parameters (electrode potential, solution concentration, volume of device, flow rates, etc.) [11-13]. In order to understand the electrode performance coupled with device performance, the system needs to be considered in terms of desalination metrics such as water recovery or salt rejection. Previously, Zhao et al. experimentally examined water recovery for a constant-current, membrane-CDI system [14, 15]. Demirer et al. experimentally investigated the trade-off between energy and water recovery [16]. Recently, Hemmatifar studied parasitic losses in CDI to optimize trade-offs between salt adsorption capacity and energy losses [17].

In this study, we developed an approach for CDI device optimization based on salt rejection. The salt rejection, SR, is used to compare the average concentration of the permeate during the desalination phase of the cycle, $\bar{c}_{out}$, to the feed concentration, c_∞ (Fig. 1b).

$$SR = 1 - \frac{\bar{c}_{out}}{c_\infty} \tag{1}$$

In order to predict salt rejection for a variety of devices, we developed a numerical simulation for flow-between CDI. We experimentally and theoretically studied the role of device specifications (feed concentration, desired effluent concentration, flow rate, volume) on design parameters (electrode type, electrode thickness, channel gap, width, length, etc.) for a continuously operating flow-between CDI system. We used vertically-aligned carbon nanotube (VA-CNT) electrodes as a simple material to obtain a device level perspective on the dynamics of a CDI device. This study focuses on constant voltage, flow-between CDI systems with adsorptive electrodes. The results presented in this work can be extended to other porous electrodes and allow for optimization of CDI devices for real-world operation.

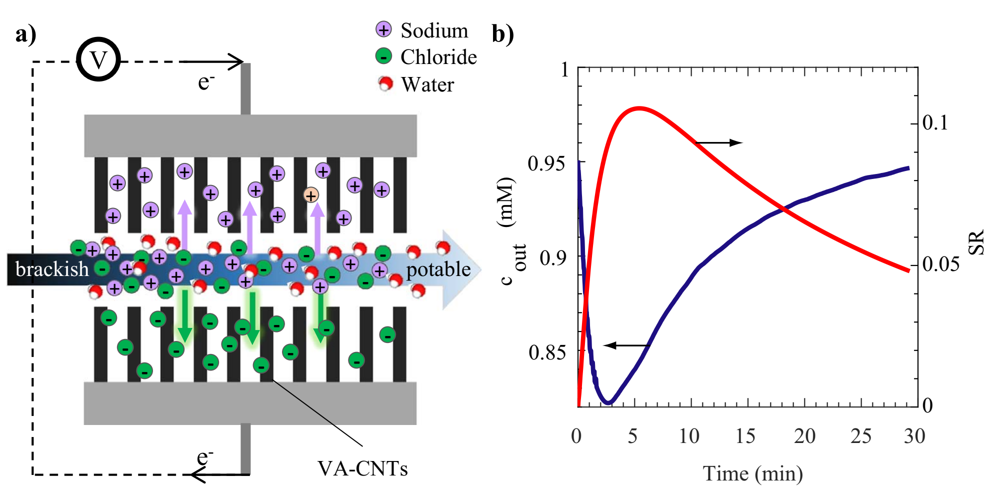

Fig. 1. CDI desalination system. a) Schematic of flow-between CDI cell and b) Salt rejection at the outlet compared with the effluent concentration during a charge cycle.