Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supporting Information: "Capacitive Deionization for Selective Removal of Nitrate and Perchlorate: Impacts of Ion Selectivity and Operating Constraints on Treatment Costs"

Steven Hand and Roland D. Cusick*

Department of Civil and Environmental Engineering

University of Illinois at Urbana-Champaign, Urbana, IL 61801-2352

Pages: 7

Figures: 3

Tables: 1

Section 1 – Supplemental Figures and Tables

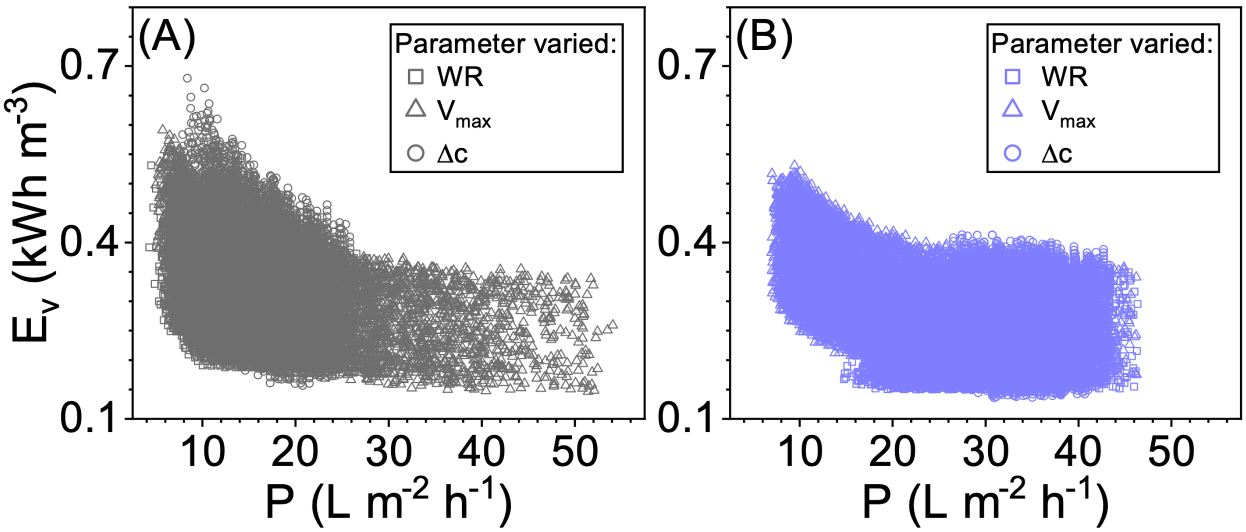

Figure S1: Individual run outputs for common metrics E_v vs P of CDI (gray, A) and MCDI (blue, B) systems as simulated across varying water recovery (square), cell voltage (triangles), and concentration reduction (circle) as detailed in Section 3.1.

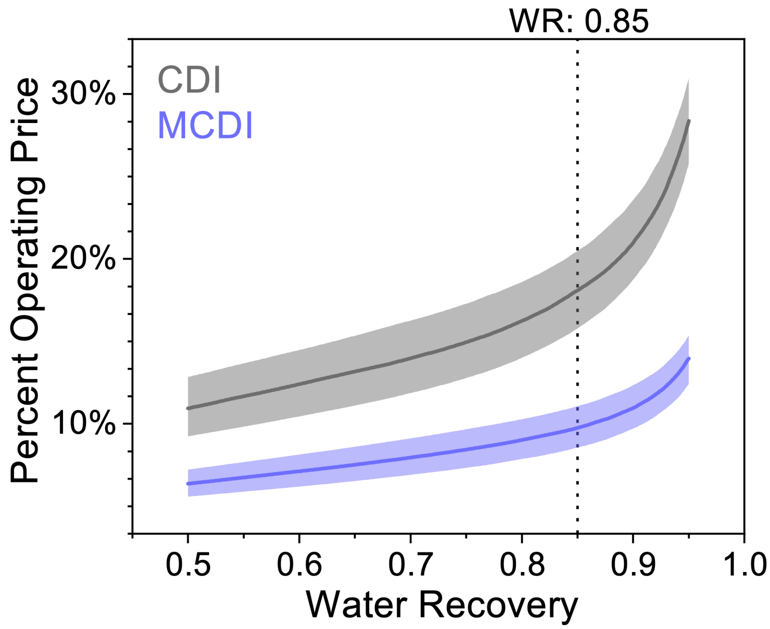

Figure S2: Operating cost as a percentage of total system cost for CDI and MCDI with increasing water recovery. The influent target ion (c_0) is fixed at 10 meq L^{-1}, removal fraction is 50%, cell voltage is 0.6 V, and ion selectivity is one. As water recovery increases beyond 0.85, operating costs exponentially increase as percent of total system costs.

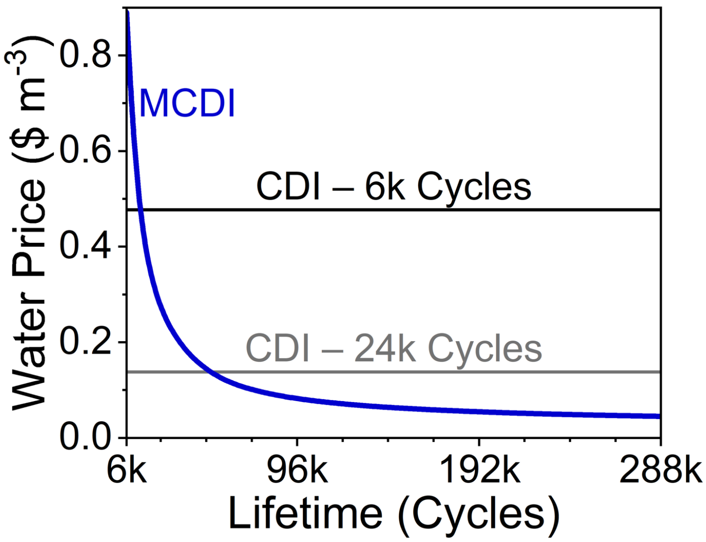

Figure S3. Median water price for MCDI system (blue) as a function of system lifetime. The influent target ion (c_0) is fixed at 10 meq L^{-1}, target ion removal is 50%, the water recovery is 0.85, cell voltage limit is 0.6 V, and ion selectivity is one. Median CDI performance under identical conditions shown at 6,000 (black) and 24,000 (grey) cycle lifetimes.

Table S1: Input parameters for NO_3^--selective CDI case studies.

Input	Value	Unit
Voltage Limit	0.6	V
Total Cycle Time	1200	s
Electrode Area	100	cm^2
Area-normalized equivalent series resistance	90	$\Omega\ cm^2$
Flow	200	$L\ s^{-1}$
Specific Capacitance	50	$F\ g^{-1}$
Current Density	5	A/m^{-2}
CDI Charge Efficiency	0.4	
Water Recovery	0.85	
Decatur		
Flow	880	$L\ s^{-1}$
Influent Concentration	2.72	$meq\ L^{-1}$
Israel		
Flow	13.3	$L\ s^{-1}$
Influent Concentration	6.35	$meq\ L^{-1}$
Spain		
Flow	206	$L\ s^{-1}$
Influent Concentration	12.73	$meq\ L^{-1}$

Section 2 – System sizing and costing equations.

$$V_m = Ri_c + \frac{i_c t_c}{C} \quad (1)$$

$$R = R_s + R_{ct} + R_i \quad (2)$$

$$t_c = tWR \quad (3)$$

$$N = \frac{(c_{in} - c_{out})QF}{i_c\, \eta_C \eta_f} \quad (4)$$

$$Q = \frac{Q_p}{WR} \quad (5)$$

$$\eta_f = \frac{2\tau_c}{t_c} \ln\left(\frac{e^{\frac{t_c}{\tau_c}} + 1}{2}\right) - 1 \quad (6)$$

$$\tau_c = \frac{V_{eff}}{Q} \quad (7)$$

$$m = \frac{t_c N}{C_g\left(\frac{V_m}{i_c} - R\right)} \quad (8)$$

$$\delta_e = \frac{m}{2\rho_e A N} \quad (9)$$

$$E_c = \frac{1}{2}(V_m + Ri_c) t_c i_c N \quad (10)$$

$$t_d = t(1 - WR) \quad (11)$$

$$i_d = \frac{i_c t_c}{t_d} \quad (12)$$

$$E_d = -\frac{1}{2}(V_m - Ri_d)t_d i_d N \quad (13)$$

$$P_{cap} = mC_c + m_b C_b + m_{ad} C_{ad} + A\left[N_m C_f + N(2C_{IEM} + C_s) + (N+1)C_{cc}\right] + WC_{bop} \quad (14)$$

$$P_{op} = (E_c + \eta_R E_d)C_e \omega + P_{lab} \quad (15)$$

List of Symbols:

A	electrode area, cm^{-2}
C	capacitance, F
C_{ad}	cost of cond. additive, $ kg^{-1}
C_b	cost of binder, $ kg^{-1}
C_{bop}	balance-of-plant costs, $ kW^{-1}
C_c	cost of carbon, $ kg^{-1}
C_{cc}	cost of current collector, $ m^{-2}
C_e	cost of electricity, $ kWh^{-2}
C_f	cost of housings/frames, $ m^{-2}
C_g	specific capacitance, F g^{-1}
C_{IEM}	cost of IEMs, $ m^{-2}
c_{in}	influent concentration, meq L^{-1}
c_{out}	effluent concentration, meq L^{-1}
C_s	cost of separator, $ m^{-2}
E_c	charging input energy, J
E_d	discharge. recoverable energy, J
F	Faraday constant
i_c	charging current density, A m^{-2}
i_d	discharging current density, A m^{-2}
m	mass of active material, kg
m_{ad}	mass of conductivity additive, kg
m_b	mass of binder, kg
N	total number of cell pairs
N_m	number of cell pairs per stack
P_{cap}	capital cost, $
P_{lab}	annual labor cost, $ yr^{-1}
P_{op}	annual operating cost, $ yr^{-1}
Q	total treatment flow, L s^{-1}
Q_p	fixed production rate, L s^{-1}
R	total resistance, Ω
R_{ct}	contact resistance, Ω
R_i	ionic resistance, Ω
R_s	setup resistance, Ω
t	total cycle duration, s
t_c	charging duration, s
t_d	discharging duration, s
V_{eff}	effective cell volume, L
V_m	voltage limit, V
W	peak power consumption, W
WR	water recovery
δ_e	electrode thickness, μm
η_C	effective charge efficiency
η_f	flow efficiency
η_R	round-trip efficiency
ρ_e	electrode density, g cm^{-3}
τ_c	cell residence time, s
ω	cycles per year, yr^{-1}