Supporting Information for

A Mathematical Model of Dynamic Behavior of Microbial Desalination Cells for Simultaneous Wastewater Treatment and Water Desalination

Qingyun Ping [†, #], Chenyao Zhang [‡, #], Xueer Chen [‡], Bo Zhang [§], Zuyi Huang [‡,*] and Zhen He [†,*]

[†] *Department of Civil and Environmental Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA*

[‡] *Department of Chemical Engineering, Villanova University, Villanova, PA 19085, USA*

[§] *Key Laboratory of Environmental Biotechnology, Research Center for Eco-Environmental Sciences, Chinese Academy of Science, Beijing 100085, China*

[#] Equal contribution

[*]Corresponding authors

Zuyi Huang: Phone (610) 519-4848, fax (610) 519-7354, email: zuyi.huang@villanova.edu

Zhen He: Phone (540) 231-1346, fax (540) 231-7698, e-mail: zhenhe@vt.edu

Number of pages: 9

Number of figures: 4

Number of tables: 2

Large MDC system setup and operation

The MDC system, consisting of 30 individual tubular MDCs hydraulically connected by the anolyte and the salt water, had a total anolyte volume of 60 L and a total desalination volume of 15 L, while the cathode compartment had a liquid volume of 30 L. Thus, the total liquid volume of the system was 105 L. The ratio between the anolyte and desalination volumes was 4:1, which was determined according to an MDC mathematical model that found that the desalination effectiveness was close to the highest at a ratio of 3-4 and further decreasing the ratio would have very minor increase in the desalination effectiveness. The individual MDC was built similarly to the one reported in a previous study.[1] A 1-m long carbon brush was inserted into the AEM tube as the anode electrode; before use, the carbon brush was pretreated according to a previous work. [2] The cathode electrode was carbon cloth coated with activated carbon powder (5 mg cm^{-2}) as a cathode catalyst;[3] the carbon cloth wrapped the CEM tube and fixed with titanium wire.

The system was operated continuously at room temperature (~ 20 °C). The anodes of the MDCs were inoculated with the mixture of aerobic and anaerobic sludge from a wastewater treatment plant (Peppers Ferry, Radford, VA, USA). The synthetic wastewater containing glucose as a carbon source was prepared as (per L of tap water): glucose, 3000 mg L^{-1}; NH4Cl, 0.15 g; NaCl, 0.5 g; $MgSO_4$, 0.015 g; $CaCl_2$, 0.02 g; KH_2PO_4, 0.53 g; K_2HPO_4, 1.07 g; yeast extract, 0.1 g; and trace element, 1 mL.[4] The salt solution was prepared by dissolving NaCl into tap water at a concentration of 35 g L-1, and fed into the desalination chambers of the MDCs as a single stream flowing through all the MDCs in series at a flow rate of HRT of 2 d. The anode and the cathode electrodes of each MDC were connected across an external resistor of 0.1 Ω to form an individual electrical circuit.

Table S1. Sensitivity measure of the top 10 ranked parameters

Rank	**Parameters**	**Descriptions**	**Sensitivity measure**
1	k_r	Parameter in Eq.13 & 15	1
2	d	Diffusion coefficient of salt in Eq. 13.	0.045
3	V_{min}	Minimum V_{oc}	0.0067
4	R_{max}	Maximum internal resistance	0.0046
5	Y_M	Mediator yield in Eq.11	0.0038
6	$k_{a,max}$	Maximum microorganism growth rate in Eq. 9	0.0038
7	$C_a(0)$	Initial concentration of anodophilic microorganism	0.0037
8	n	Electrons transferred per mol of mediator	0.0017
9	$C_{a,max}$	Maximum attainable concentrations for anodophillic microorganism	0.00028
10	M_{total}	Total mediator fraction	0.00014

Table S2. Parameters used in the model.

Parameters	Description	Values
$k_{s,a,max}$	Maximum substrate consumption rates by anodophilic microorganisms	5.32 mg-S·mg-a^{-1}·day^{-1}
$k_{s,m,max}$	Maximum substrate consumption rates by methanogenic microorganisms	8.20 mg-S·mg-a^{-1}·day^{-1}
K_a	half-saturation concentrations for the anodophillic microorganism	20 mg-S·L^{-1}
K_m	half-saturation concentrations for the methanogenic microorganism	80 mg-S·L^{-1}
K_M	half-saturation concentrations for the redox mediator	0.2* M_{total} mg-M·mg-a^{-1}
$k_{\alpha,x}$	the steepness factors for anodophillic microorganism	0.04 L·mg-a^{-1}
$k_{m,x}$	the steepness factors for methanogenic microorganism	0.04 L·mg-m^{-1}
$C_{\alpha,max}$	maximum attainable concentrations for anodophillic microorganism	512.5 mg-a·L^{-1}
$C_{m,max}$	maximum attainable concentrations for methanogenic microorganism	525 mg-m·L^{-1}
$k_{a,max}$	maximum microorganism growth rates for anodophillic microorganism	0.197 day^{-1}
$k_{m,max}$	maximum microorganism growth rates for methanogenic microorganism	0.10 day^{-1}
M_{total}	Mediator fraction	0.05 mg-M·mg-x^{-1}
Y_M	the mediator yield	6.14 mg-M·mg-S^{-1}
γ	Mediator molar mass	663,400 mg-M·mol$_{mediator}^{-1}$
n_e	Electrons transferred per mol of mediator	2 mole^{-1}·mol$_{mediator}^{-1}$
F	Faraday constant	96,485 A·s·mole^{-1}
d	the membrane salt transfer coefficient	0.029 day^{-1}
k_r	Parameter in Eq.13 & 15	0.082 L·mg-a^{-1}
R	Ideal gas constant	8.314472 J·K^{-1}·mol^{-1}
T	MDC temperature	298.15 K

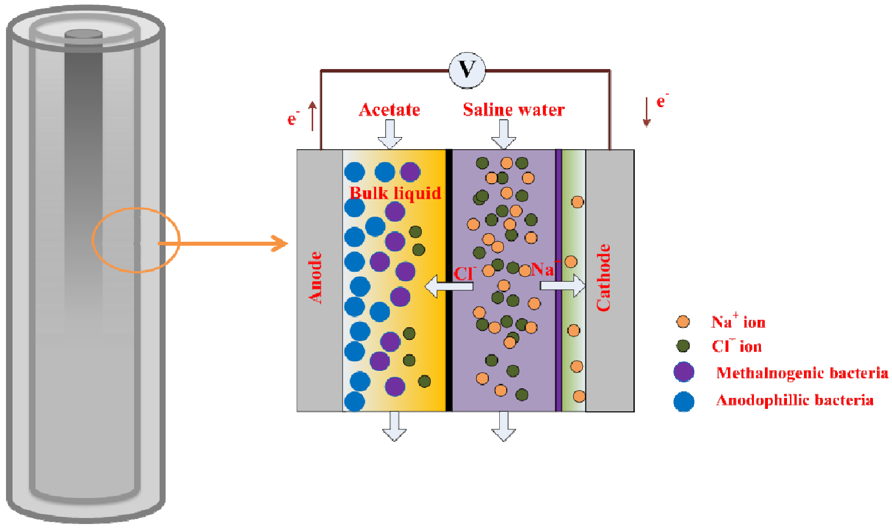

Figure S1. Schematic diagram of a tubular microbial desalination cell

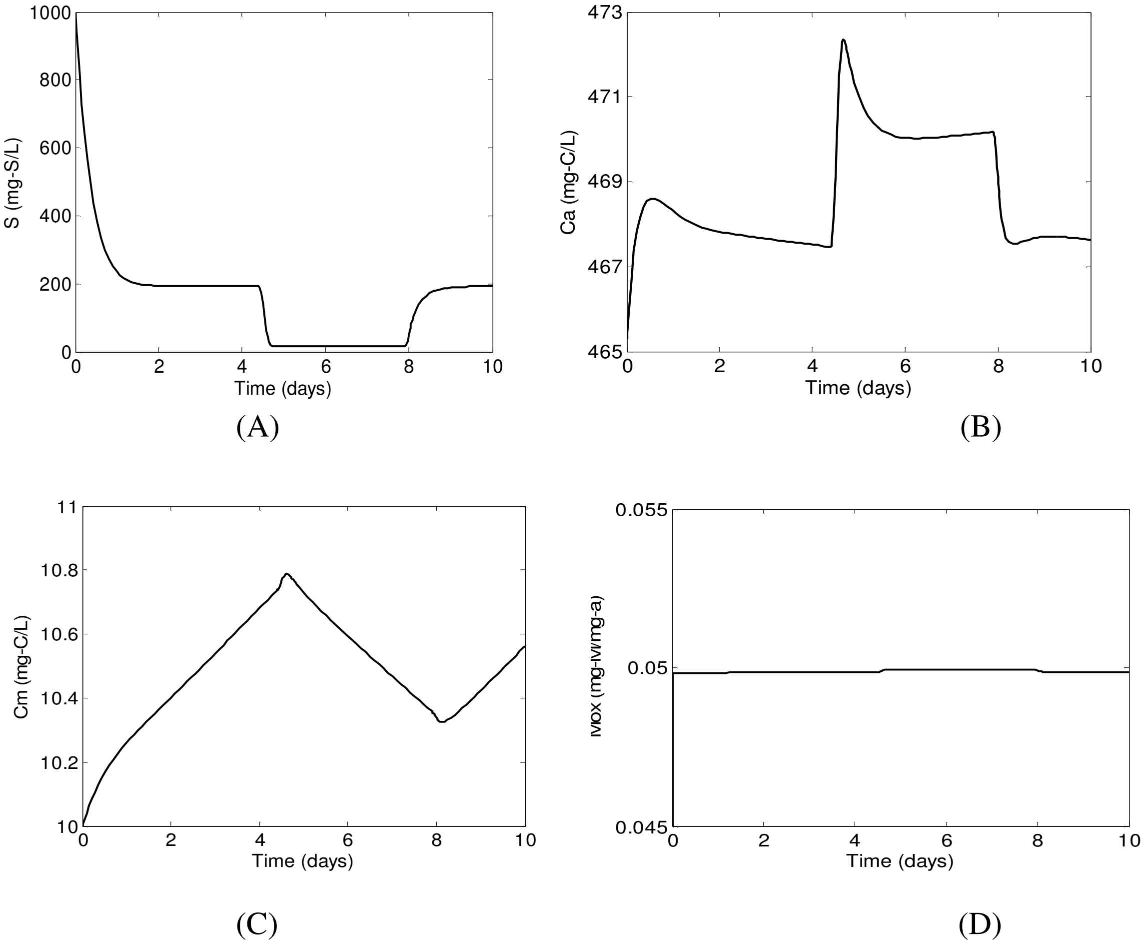

Figure S2. The simulation results when the anode influent feeding rate was changed from 0.5 to 0.2, and then back to 0.5 mL·min^{-1}: A) substrate concentration, B) the concentration of anodophillic microorganisms, C) the concentration of methanogenic microorganisms, and D) the oxidized mediator fraction per anodophillic microorganism.

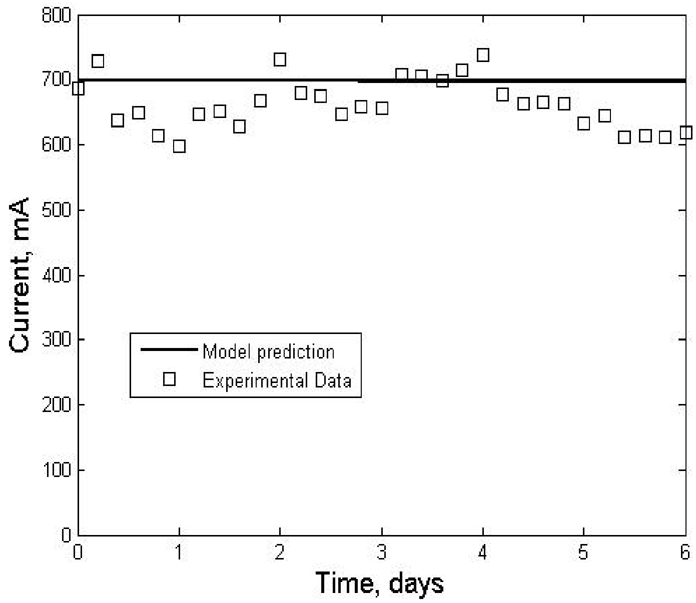

Figure S3. Experimental data and model prediction of the current generation of the large-scale MDC system

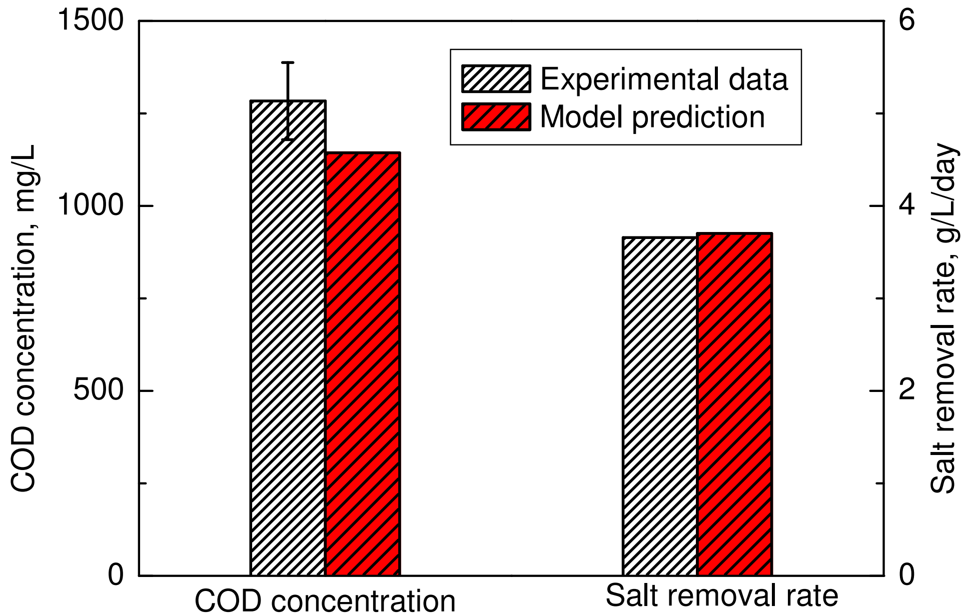

Figure S4. Experimental data and model prediction of the anode effluent COD concentration and salt removal rate of the large-scale MDC system

References

1. Jacobson, K. S.; Drew, D.; He, Z., Use of a liter-scale microbial desalination cell as a platform to study bioelectrochemical desalination with salt solution or artificial seawater. *Environ. Sci. Technol.* **2011,** *45*, 4652-4657.
2. Wang, X.; Cheng, S.; Feng, Y.; Merrill, M. D.; Saito, T.; Logan, B. E., Use of carbon mesh anodes and the effect of different pretreatment methods on power production in microbial fuel cells. *Environ. Sci. Technol.* **2009,** *43*, 6870-6874.
3. Zhang, F.; Ge, Z.; Grimaud, J.; Hurst, J.; He, Z., Long-term performance of liter-scale microbial fuel cells installed in a municipal wastewater treatment facility. *Environ. Sci. Technol.* **2013,** *47*, 4941-4948.
4. Angenent, L. T.; Sung, S., Development of anaerobic migrating blanket reactor (AMBR), a novel anaerobic treatment system. *Water Res.* **2001,** *35*, 1739-1747.