Supplementary Information

for

The role of nanoscale morphology on the efficiency of solvent-based desalination method

Peerless, James S.[1]; Gulyuk, Alexey V.[1]; Milliken, Nina J. B.[1]; Kim, Gyu Dong[2]; Reid, Elliot[3]; Lee, Jae Woo[4]; Kim, Dooil[5]; Hendren, Zachary[6]; Choi, Young Chul[7]; Yingling, Yaroslava G.[1]*

[1.] *Department of Materials Science and Engineering, North Carolina State University, 911 Partners Way, Raleigh, NC, 27695, United States*
[2.] *Center for Technology Advancement & Commercialization, RTI International, 3040 Cornwallis Road, Research Triangle Park, NC 27709, United States*
[3.] *School of Civil and Environmental Engineering, Georgia Institute of Technology, North Ave NW, Atlanta, GA, 30332, United States*
[4.] *Department of Environmental Engineering, Korea University, Sejong Campus, 2511 Sejong-ro, Sejong 339-700, Korea*
[5.] *Department of Civil and Environmental Engineering, Dankook University, 152, Jukjeon-ro, Suji-gu, Yongin, Gyeonggi-do, 16890, Korea*
[6.] *A.R. Smith Department of Chemistry & Fermentation Sciences, Appalachian State University, 73 Rivers Street, Boone, NC 28608, United States*
[7.] *Research & Development Center, Saudi Aramco, P.O. Box 12232, Dhahran, 31311, Saudi Arabia*

*Corresponding Author: Address correspondence to yara_yingling@ncsu.edu

Contents

S1. Additional Background Information

Some additional explanations of the steps of solvent-based desalination (SBD) method that serves as a foundation in the experimental setup utilized in our work.

SBD is identified as solvent extraction desalination (SED) and temperature swing solvent extraction (TSSE), that, combined, leverage the temperature-dependent solubility of the solvent. Consecutively this allows to extract clean water from a brine solution.

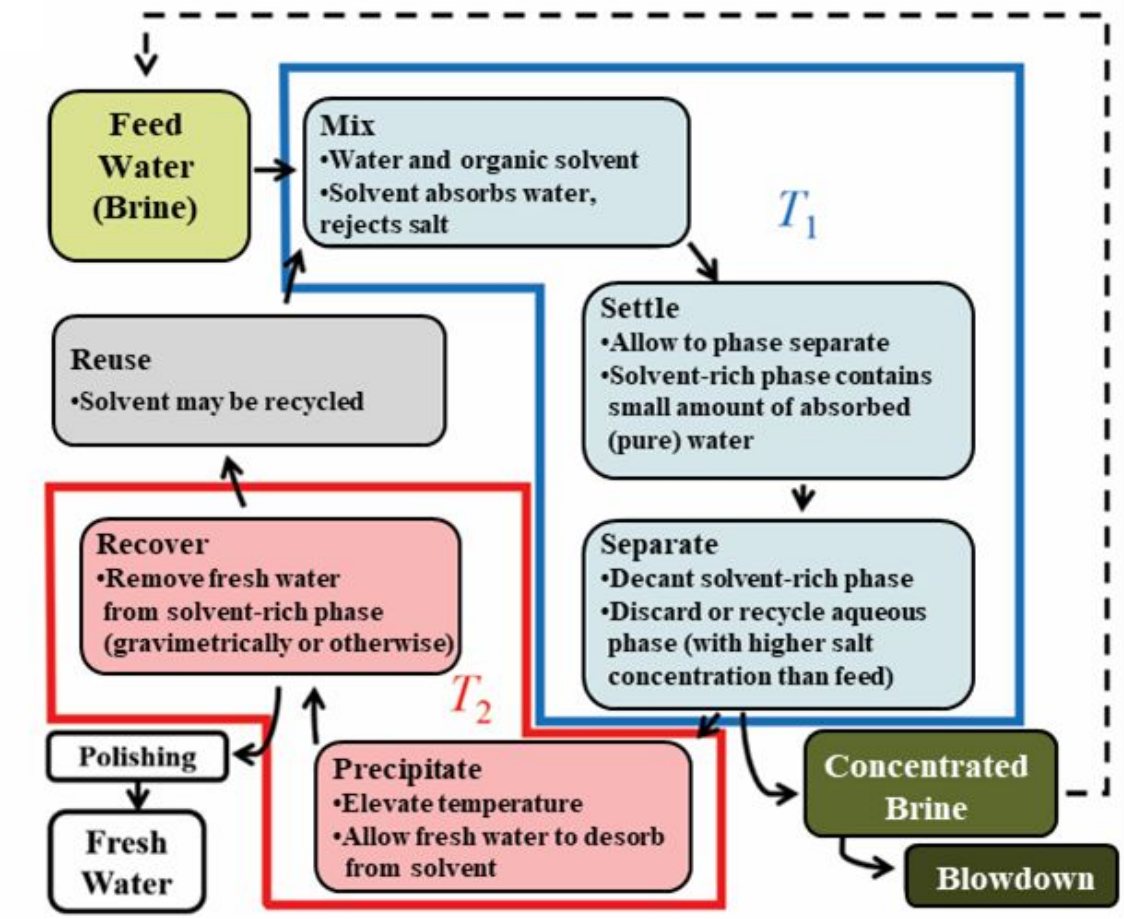


Figure S1. Diagram of the solvent-based desalination (SBD) process to extract water from a brine solution using an organic solvent with a temperature-dependent water solubility.

S2. Additional Simulation and Experimental Data

Table S1. Details from MD simulations. Average Volume reported for last ns of simulation ± standard deviation in that time.

Solvent	Water Molecules (#)	Total Atoms (#)	Average Volume ($Å^3$)
7A	6,935	45,953	449,300 ± 2,280
8A	8,695	54,251	523,100 ± 6,570
AMH	9,567	56,869	559,780 ± 784
BPA	8,256	49,922	509,590 ± 821
DBA	9,201	55,771	567,890 ± 829
DBE	9,146	54,612	569,240 ± 854
DPA	7,162	43,624	447,530 ± 772
EHA	8,852	54,720	539,580 ± 765
HMA	9,093	52,431	530,360 ± 779
PBA	8,175	49,679	507,680 ± 804

Table S2. Details of the available experimental data. Averages and standard errors reported for two rounds of tests performed.

Solvent	**Water recovery (%)**				**Cl Rejection (%)**			
	1	2	Average	STDEV	1	2	Average	STDEV
1-Heptylamine (7A)	28.7	30.5	29.6	1.27	31.4	33.3	32.35	1.34
Octylamine (8A)	26.1	25.3	25.7	0.57	24.1	25.6	24.85	1.06
Dibutylamine (DBA)	3.2	4.5	3.85	0.92	99.2	98.9	99.05	0.21
Dipropylamine (DPA)	9.8	10.3	10.05	0.35	93.8	95.6	94.7	1.27
2-Ethylhexylamine (EHA)	10.7	10	10.35	0.49	55	58	56.5	2.12
Propylbutylamine (PBA)	5.3	4.9	5.1	0.28	98.8	97.5	98.15	0.92

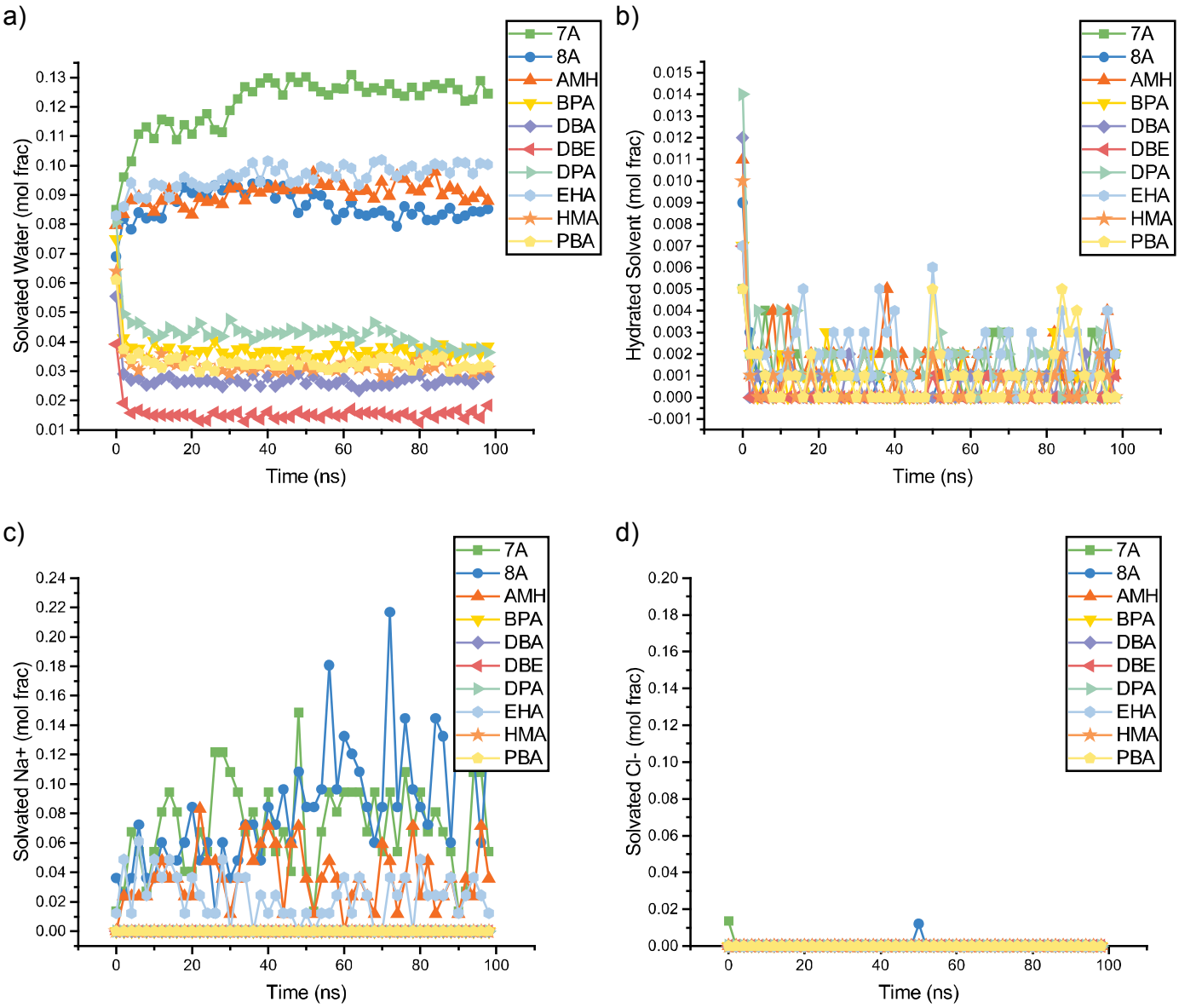
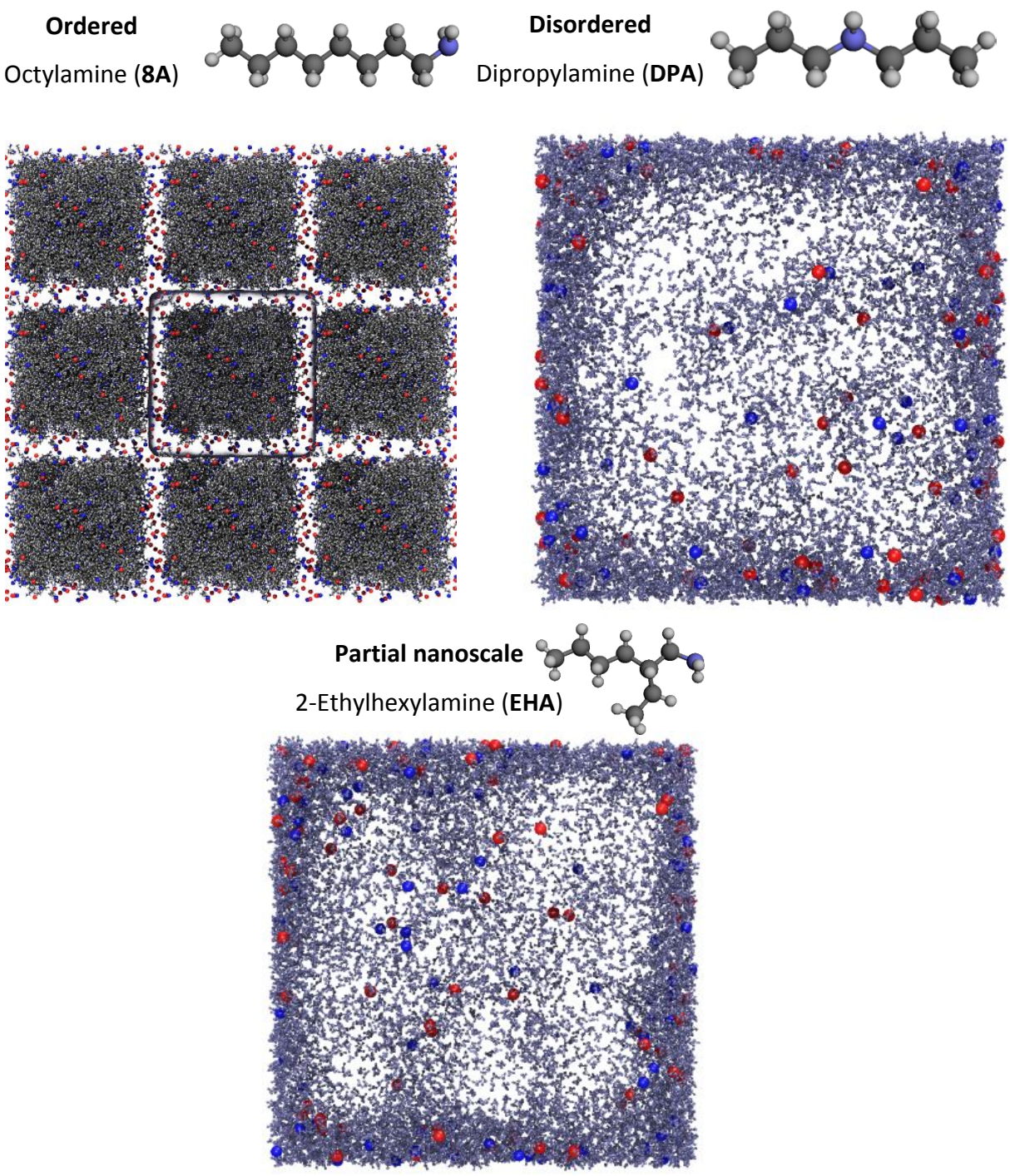
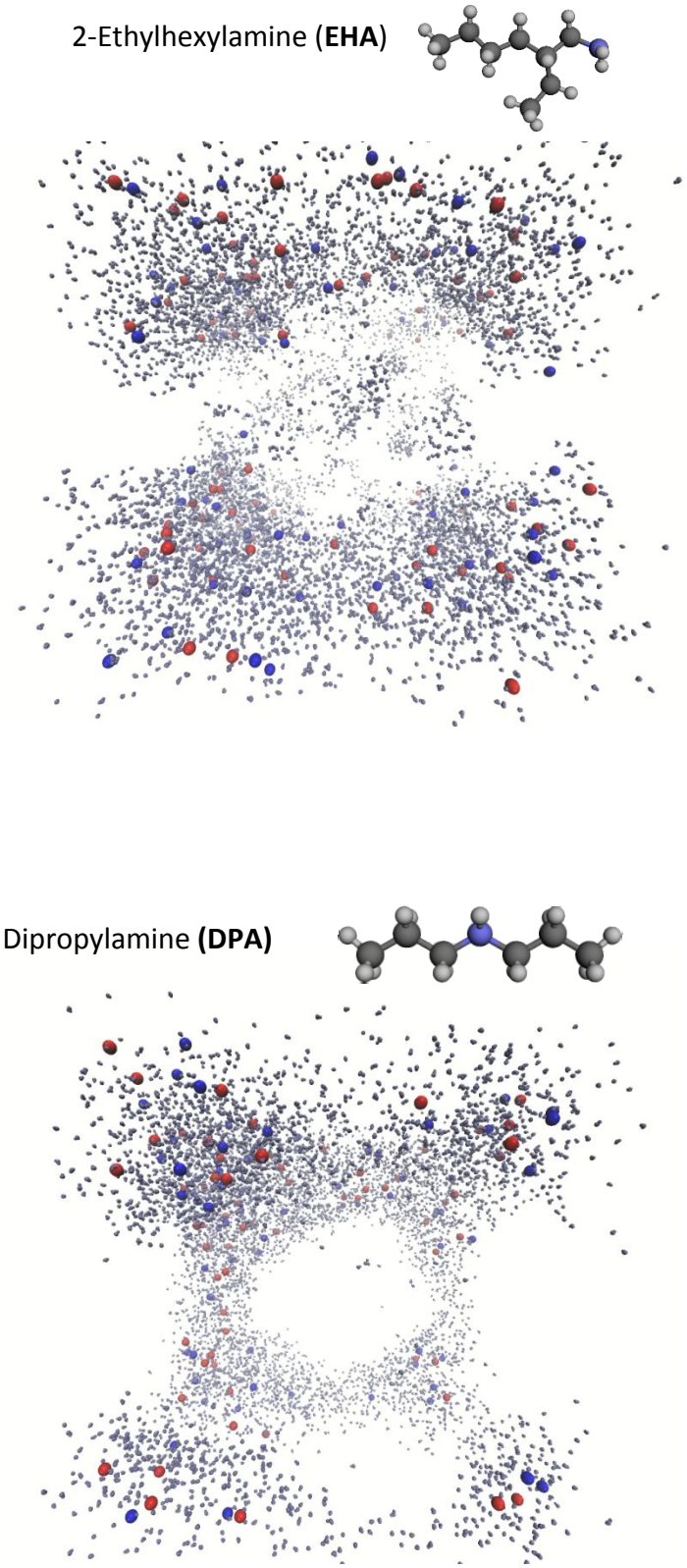


Figure S2. Measurements of a) solvated water, b) hydrated solvent (solvent leftover), c) solvated Na^+, and d) solvated Cl^- from last 100ns of MD simulations shown over time. Units of concentration (molar fractions) defined as the number of moles of a solvated agent divided by the total molar number of a solution tested. All measurements performed as described in Materials and Methods sections.

As it can be observed, the results show notable difference between solvation of Na^+ and Cl^- ions. This can be explained as follows. Based on the ion size, comparing Na^+ and Cl^-, the Cl^- ion is too large to effectively penetrate the solvated phase in the given simulation time. Though given that a bulk system would have charge neutrality, the Cl^- ions around follow along in the separation process thus making the system not being hydrated efficiently. To better visualize the process of phase formation and ion solvation, we added movies below (Movie S1 and Movie S2).



Movie S1. Phase separation dynamics representing three observed mechanisms: ordered phase separation (left), disordered phase separation (right), and partial nanoscale phase separation (bottom).



Movie S2. Disordered phase separation dynamics. Representatve compilation of snapshots for 2-Ethylhexylamine (top) and Dipropylamine (bottom). Insets show the structure of a solvent molecule.