Supporting Information

Using UCST Ionic Liquid as a Draw Solute in Forward Osmosis to Treat High-Salinity Water

*Yujiang Zhong, Xiaoshuang Feng, Wei Chen, Xinbo Wang, Kuo-Wei Huang, Yves Gnanou, Zhiping Lai **

Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, 23955-6900

Corresponding author:

E-mail: Zhiping.lai@kaust.edu.sa

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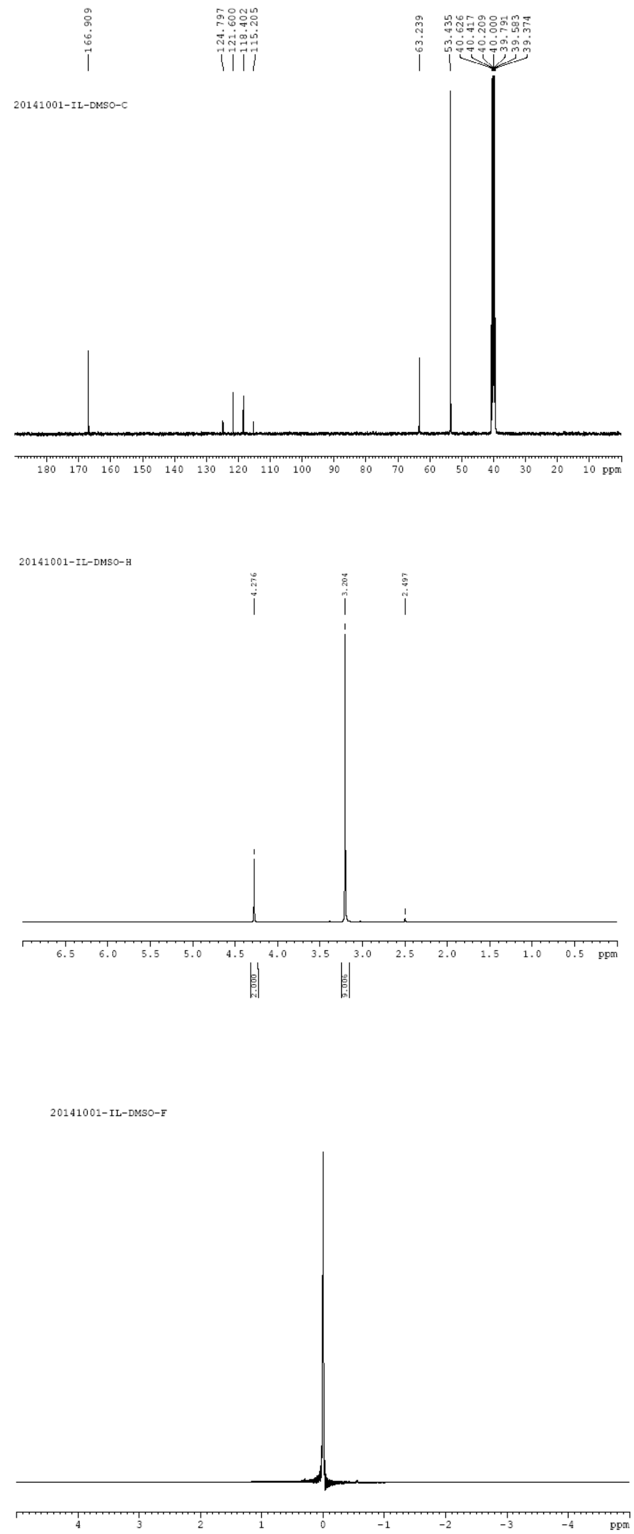

Figure S1. a) ^{13}C NMR of [Hbet][Tf2N]; b) ^{1}H NMR of [Hbet][Tf2N] and c) ^{19}F NMR of [Hbet][Tf2N].

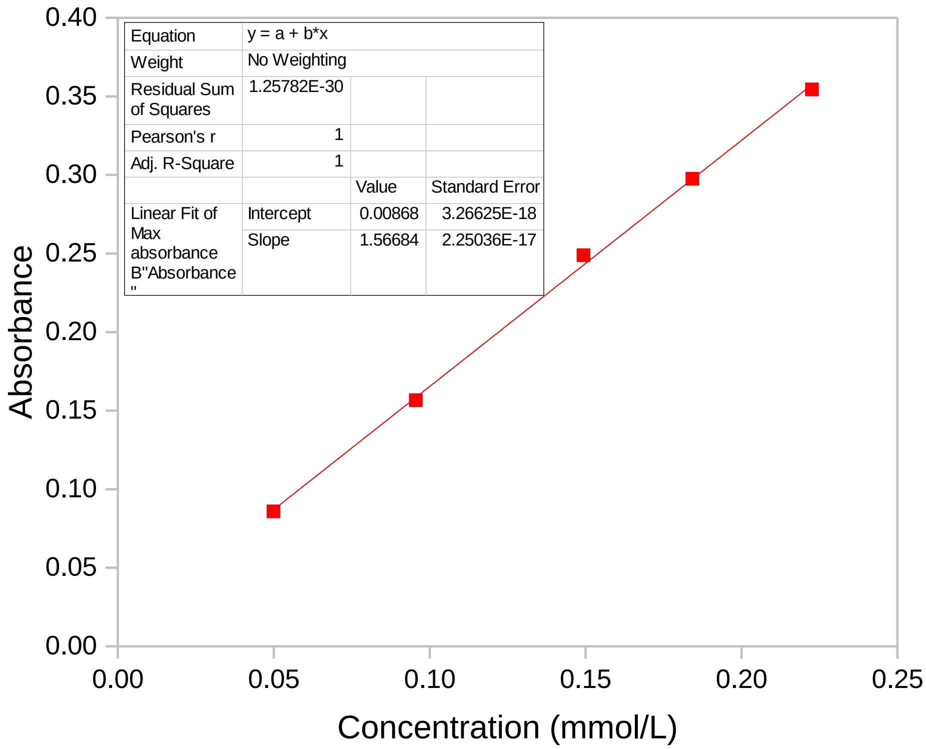

Figure S2. Linear relationship of the absorbance in λ_{Max} with different concentration of [Hbet][Tf_2N].

S3: Energy calculation of different seawater desalination processes using UCST ILs as draw solutes.

According to the experimental results listed in Table 1 in the manuscript, in the case of seawater treatment (0.6 M NaCl as feed solution), the produced water contains 0.079 mol/L NaCl which equals to 4621.5 mg/L (ppm) NaCl, and 0.3475 mol/L IL that is equivalent to 20328.8 ppm NaCl. There are several methods to polish this water. The seawater concentration is around 35,000 ppm NaCl. In order to make a comparison, several combination of treatment methods were studied, and the results were listed in Table S1. In all combinations, the capacity were fixed at 100 m^3/h. The SWRO and other polishing processes were operated at 23 ℃. Case #1 is a one-step SWRO. The simulation tool Toray DS2 was used to simulate the SWRO process. Among the global available SWRO membrane elements in Toray DS2 system, TM 820V-440 was selected because of the highest nominal flow rate per unit area, and Isobaric Device ERI was selected as the energy recovery device. The operation pressure is 79.48 bar and water recovery is 50%. In case #2, SWRO (TM 820V-440, ERI) was used to treat the produced water of the thermal FO process. The produced water was considered as a solution of NaCl with the same total molar concentration, i.e. the sum of NaCl and IL concentration, as 24900 ppm NaCl, since there is seldom study of IL solution treatment by SWRO. The operation pressure is 48.77 bar and water recovery is 50%. In case #3, NF was used to polish the produced water of FO process. The operation conditions were based on reported results in literature,[1] where a NF-270 membrane was used; operation pressure was 35 bar; IL rejection was 95.2%, NaCl rejection was 50%, and water recovery was 80%. In case #4, a BWRO process was used to polish the produced water. The BWRO membrane element TM-710D was used because it has the same performance parameters as the flat BWRO membrane used in the FO process. The BWRO process with a equivalent NaCl 4621 ppm was also simulated by Toray DS2. The water recovery was 85%, and operation pressure was 19.0 bar. The IL concentration was not included in the simulation. Since the NF process could reject 95% IL, hence the tighter BWRO membrane was considered as a filter of IL. The IL rejection was set as 99.97%, which was the lowest experimental result of FO. In case #2 and #4, the feed solution containing high concentration of IL may cause fouling problems, while the final produced water quality in case #3 was still not good enough. Therefore, a finer process case #5 was also considered. In case #5, the produced water of FO process was first treated with a NF process to remove almost all the IL and half of NaCl. Then the solution that contained very little IL and about 2300 ppm NaCl was treated by BWRO (TM-710D). The water recovery was 89%, and the operation pressure was 16.1 bar. The IL rejection was also set as 99.97%. In the final produced water the IL concentration was much smaller than case #4, so it was neglected. [Hbet][Tf_2N] can also draw water from high salty water that SWRO can't work. The common methods to treat high salty water are traditional thermal technologies like multiple effect distillation (MED) and multi-stage flash (MSF). The unit thermal energy requirement of these technologies is in the range of 60~80 kWh/m^3, which is much higher than that of the thermal FO process. Due to the low operation temperature, solar energy and waste heat could be good heat sources, which could be very cheap.

In the energy calculation of seawater treatment by thermal FO processes, the batch mode was considered. With different starting feed to draw weight ratio, the water recovery and the final equilibrium concentration were different, as shown in Figure 7. The smaller the ratio, the higher are the water recovery and the final equilibrium concentration. The upper limit of water recovery is about 80%. When the feed to draw weight ratio attained 1:10, the water recovery was close to 80%. The seawater heat capacity is about 4.0 kJ/kg/K, and the heat capacity of [Hbet][Tf_2N] is about 1.468 kJ/kg/K.[2] In the thermal energy consumption calculation, the feed to draw weight ratio was set as 1:1, and the water recovery was 63.8%. A heat exchanger was considered here. Based on the calculation by the Model 02626-05 (73 Series Sanitary Double Tubesheet HX, 30 Inch Tube Bundle, provided by EXERGY LLC), about half of the heat energy could be reused. The thermal energy used in the FO process per unit produced water was listed in the last column of Table S1.

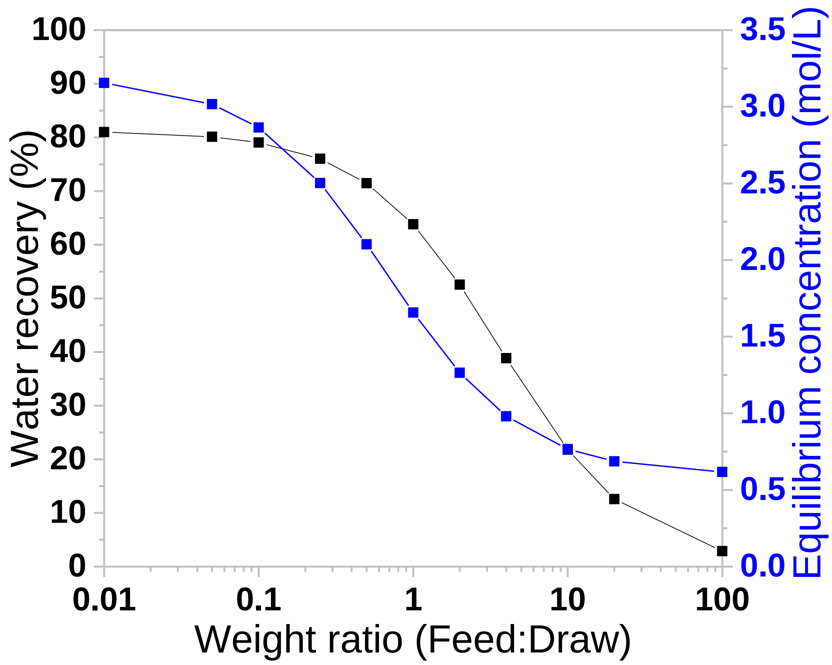

Figure S3. Water recovery and final equilibrium concentration in the FO process that 3.2 M [Hbet][Tf2N] as draw solution and 0.6 M NaCl (seawater) as feed solution at 60 ℃ with different weight ratio of feed to draw.

Table S1. Comparison of different seawater treatment processes.

No.	Processes	Final Water Quality		Electrical energy consumption (kWh/m^3)	Thermal energy consumption (kWh/m^3)
		NaCl (ppm)	IL (mol/L)		
1	SWRO	213.5	\	2.964	\
2	FO + SWRO	161.5	\	1.903	44.15
3	FO + NF	2310.75	0.017	1.215	44.15
4	FO + BWRO	117.5	0.0000382	0.78	44.15
5	FO + NF + BWRO	62.58	\	1.845	44.15

REFERENCE

1. Fernández, J. F.; Bartel, R.; Bottin-Weber, U.; Stolte, S.; Thöming, J., Recovery of Ionic Liquids from Wastewater by Nanofiltration. *J. Membr. Sci. Technol.* **2011**, S:4, 1-8.
2. Jagadeeswara, R. C.; Venkata, K. R.; Venkatesan, K. A.; Nagarajan, K.; Srinivasan, T. G., Thermochemical properties of some bis(trifluoromethyl-sulfonyl)imide based room temperature ionic liquids. *J. Therm. Anal. Calorim.* **2009,** *97*, (3), 937-943.