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Advancing the Productivity-Selectivity Trade-off of Temperature Swing Solvent Extraction Desalination with Intermediate-Step Release

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IR) over a conventional (c-TSSE) single-step operation. TSSE-IR demonstrated superior performance in the hypersaline desalination of 1.0 M NaCl brines for three amines with distinct water and salt partitioning behaviors: diisopropylamine, triethylamine, and tertoctylamine. The astute introduction of the intermediate temperature step in TSSE-IR dramatically improves salt rejection while minimizing the sacrifices in water recovery yields. We show that



the intermediate step does not introduce additional solvent loss compared with c-TSSE operations with the same extraction temperature for any of the three solvents examined. TSSE-IR is demonstrated to advance the productivity-selectivity trade-off that constrains c-TSSE. Finally, Hunter-Nash analysis conducted on diisopropylamine-H₂O-NaCl ternary diagrams exhibits good agreement with experimental TSSE-IR results, offering a reliable platform for modeling intermediate-step release performance and informing process design. This study establishes the potential of TSSE-IR to expand the spectrum of viable solvents for hypersaline desalination to include greener chemicals that exhibit high water recovery yields but low selectivities in c-TSSE.

KEYWORDS: Temperature swing solvent extraction, Desalination, Hypersaline brines, Thermally switchable solvents, Productivity-selectivity trade-off, Hunter-Nash analysis

INTRODUCTION

Desalination is an increasingly attractive option for the management of hypersaline brines, i.e., aqueous streams with >70,000 ppm total dissolved solids.^{1,2} These brines originate from a wide range of sources, including produced water from oil and gas extractions, mining operations, geological carbon sequestration sites, inland desalination concentrate, and landfill leachate.^{1,3-7} Due to their very high salt concentrations and presence of additional pollutants, proper management is required to avoid damage to local ecosystems and water sources from untreated discharge.^{2,3,6} Desalination reduces the brine volume, thus lowering costs and environmental impacts associated with final disposal, while simultaneously producing water for fit-for-purpose reuse applications.^{8,9} However, traditional desalination technologies face considerable technical challenges in high-salinity environments. Hypersaline feeds generally contain mineral scalants that rapidly deteriorate the performance of membrane-based processes, such as reverse osmosis.^{10,11} Evaporative desalination techniques, such as brine concentrators and brine crystallizers, are inherently energyintensive due to the high enthalpy of vaporization of water and low thermodynamic efficiencies.^{1,12}

Temperature swing solvent extraction (TSSE) is a membrane-less and nonevaporative approach for hypersaline desalination.^{13–16} In TSSE, a solvent with thermally switchable hydrophilicity extracts water from a brine feed, whereas salt ions are largely rejected by the low-polarity solvent.^{15,17-19} The water-in-solvent extract is brought to a disengagement temperature, where the solvent is in its more hydrophobic state and a product water stream demixes from the solvent. The regenerated solvent can be decanted and recycled back into the process. Because there are neither solid-liquid interfaces nor phase changes in TSSE, the technique sidesteps problems

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associated with mineral scaling and large vaporization enthalpies, respectively. Additionally, the moderate temperature swings utilized make TSSE compatible with sustainable low-grade heat sources. However, our recent study showed that TSSE performance is constrained by an inherent trade-off between water productivity and selectivity for water over salt: tuning the operating temperature to achieve higher water recovery yields unavoidably occurs with worsened salt rejection.²⁰

In this study, we demonstrate improved productivityselectivity performance of the temperature swing solvent extraction with intermediate-step release (TSSE-IR) for the desalination of hypersaline brines. In TSSE-IR, the water-laden organic phase is brought to an intermediate temperature after the initial extraction step. Salt preferentially disengages from the organic phase at this intermediate temperature, and the remaining organic extract is physically separated from the secondary raffinate before being brought to the final disengagement temperature. Water recovery yield and salt rejection performance of TSSE-IR are evaluated against conventional TSSE (c-TSSE) for three distinct amine solvents. Potential contribution of the intermediate step in TSSE-IR to amine loss is assessed and confirmed to be insignificant. Productivity-selectivity trade-off performance for TSSE-IR is benchmarked against c-TSSE. Finally, Hunter-Nash analysis is conducted on ternary phase diagrams to provide a theoretical basis for the enhanced TSSE-IR performance. Practical implications of this innovative approach for expanding the spectrum of viable solvents for desalination are discussed.

METHODS AND MATERIALS

A detailed description of the materials and methods can be found in the Supporting Information and is briefly presented here.

TSSE Intermediate-Step Release Experiments. Thermally switchable solvents of diisopropylamine (DIPA), triethylamine (TEA), and tert-octylamine (TOA) were evaluated for TSSE-IR desalination of 1.0 M NaCl brines (Figure 1). Equal weights of solvent and brine were continuously stirred for 10 min, followed by 5 min of gravitational settling, at a low temperature, $T_{\rm L}$, of 15 °C (Step I). After equilibration, the water-laden solvent phase was physically separated from the biphasic mixture, and the remaining dewatered aqueous phase is designated as the first raffinate, R_I. The solvent extract was then equilibrated at an intermediate temperature, T_{IR} , of 30 °C for at least 45 min (Step II). The mixture phase-separates, and the resulting water-in-solvent extract was isolated, with the leftover aqueous phase designated as the second raffinate, R_{II}. The final extract was equilibrated at a high temperature, $T_{\rm H}$, of 70 °C for no less than 45 min (Step III), culminating in a demixed product water that was decanted and a regenerated solvent. Masses and compositions of both phases of the biphasic mixtures at each step were analyzed (details in the Supporting Information).

RESULTS AND DISCUSSION

TSSE-IR Can Drastically Improve Salt Rejection. TSSE-IR desalination performance was evaluated for 1.0 M NaCl brine feeds with thermally switchable solvents of diisopropylamine (DIPA), triethylamine (TEA), and *tert*-octylamine (TOA). DIPA and TOA were chosen, in particular, for their relatively low salt rejections in conventional single-stage pubs.acs.org/journal/estlcu



Figure 1. Schematic illustrating the working principles of temperature swing solvent extraction with intermediate-step release (TSSE-IR). A thermally switchable amine solvent selectively extracts water from the saline feed at a low temperature, $T_{\rm L}$ (Step I). Because the salt content of the organic extract is more sensitive to changes in temperature than the water content, salt preferentially disengages at temperature $T_{\rm IR}$ of the intermediate step (Step II). The remaining organic extract is brought to a high temperature, $T_{\rm H}$, to disengage the final product water (Step III). As salt is selectively expelled in the intermediate raffinate, overall salt rejection is improved. Yellow shading of the schematic highlights the additional intermediate step of TSSE-IR relative to standard operation. Darker shades of blue represent aqueous phases with higher concentrations of salt, and darker shades of orange represent organic phases with lower water contents.

operations at $T_{\rm L} = 15$ °C. Chemical structures of the solvents are presented in Figure S1 of the Supporting Information. Low and intermediate step temperatures ($T_{\rm L}$ and $T_{\rm IR}$, respectively) of 15 and 30 °C were utilized. For comparison, the performance of conventional TSSE (c-TSSE) with $T_{\rm L}$ s of 15 and 30 °C was also assessed. A final disengagement temperature, $T_{\rm H}$, of 70 °C was used for both the TSSE-IR and c-TSSE experiments. Salt rejection (*SR*), defined as the percentage reduction in salt concentration from the initial brine feed to the product water, is presented for single extraction cycles of TSSE-IR and c-TSSE in Figure 2A.

TSSE-IR produced $3.2\times$, $1.1\times$, and $1.8\times$ improvements in salt rejections compared to c-TSSE with $T_{\rm L}$ = 15 °C for DIPA, TEA, and TOA, respectively. In particular, the enhancements are considerably more marked for DIPA and TOA, which have very poor salt rejection capabilities at $T_{\rm L}$ = 15 °C. TEA already has high salt rejections in c-TSSE operation with $T_{\rm L}$ = 15 °C; the addition of the intermediate step would be more advantageous for operations with lower $T_{L}s$, where SR will worsen.²⁰ For all three solvents, salt rejections are statistically indistinguishable (p > 0.05, Table S1 of the Supporting Information) between TSSE-IR and c-TSSE with $T_{\rm L}$ = 30 °C (filled and hatched columns, respectively). Salt contents of organic phases are more sensitive to changes in temperature than water contents (illustrated by results for DIPA and a 4.0 M NaCl brine in Figure S2 of the Supporting Information). Consequently, salt preferentially disengages from the water-in-



Figure 2. (A) Percentage salt rejection, *SR*, and (B) water recovery yield, *Y*, for 1.0 M NaCl brine feeds and amine solvents diisopropylamine, triethylamine, and *tert*-octylamine (DIPA, TEA, and TOA, respectively). For each amine, c-TSSE with T_L values of 15 and 30 °C (open and hatched columns, respectively) are compared to TSSE-IR with $T_L = 15$ °C and $T_{IR} = 30$ °C (filled columns). All three operations utilize $T_H = 70$ °C. For all three solvents, differences in salt rejections for TSSE-IR and c-TSSE with $T_L = 30$ °C are not statistically significant (p > 0.05). Batch equilibrium experiments are performed with equal weights of feeds and solvents. Data and error bars are means and one standard deviation, respectively, from duplicate experiments.

solvent extract at the intermediate temperature step. TSSE-IR is thus able to drastically improve salt rejection compared to c-TSSE with $T_{\rm L}$ = 15 °C.

Sacrifices in Water Recovery Yield Are Mitigated. Water recovery yield, *Y*, defined as the mass ratio of water in the product stream to water in the initial saline feed, is presented in Figure 2B for single extraction cycles (note that in actual continuous operations, a solvent:feed mass ratio >1 can be utilized to achieve higher Ys).¹⁵ Conventional TSSE with T_L = 15 °C (open columns) demonstrated the highest recovery yields, followed by TSSE-IR and then c-TSSE with T_L = 30 °C (filled and hatched columns, respectively). Because the extraction step temperature is identical, the same amount of water is initially extracted in TSSE-IR as c-TSSE with T_L = 15 °C. For TSSE-IR, a portion of this extracted water disengages from the extract during the intermediate step when the temperature is raised to $T_{\rm IR}$ = 30 °C, eventually resulting in a lower Y relative to this conventional TSSE operation.

However, the water recovery yield is greater for TSSE-IR compared to c-TSSE with $T_{\rm L}$ = 30 °C. Salt ions do not favor partitioning into the low-dielectric environment of the amine solvents (dielectric constants of 3.04 and 2.43 for DIPA and TEA,^{21,22} respectively, and measured to be 3.52 for TOA) and are, hence, mostly retained in the aqueous phase.^{15,17-19,23} Therefore, the ratio of salt to water extracted at $T_{\rm L}$ = 15 °C is considerably lower compared with the salt concentration of the initial brine feed (1.0 M NaCl). When amine-water-salt systems are equilibrated to form biphasic mixtures, lower salt to water ratios result in higher fractions of water in the extract.¹⁵ In addition, the proportion of organic solvent phase to aqueous phase of the biphasic mixtures is drastically higher in the intermediate step of TSSE-IR than the extraction step of c-TSSE (only a fraction of the initial feed is extracted, and only a portion of the extracted water is released in the intermediate step of TSSE-IR). These two factors allow more water to be retained by the solvent in the intermediate step of TSSE-IR than extracted in c-TSSE with $T_{\rm L}$ = 30 °C, yielding greater Y for TSSE-IR at the end of the cycles. The trends in SR and Y between TSSE-IR and c-TSSE are observed for all three amine solvents despite differences in structure and thermochemical properties. Fine-tuned selection of $T_{\rm IR}$ within the temperature range of $T_{\rm L}$ and $T_{\rm H}$ can allow for further optimization between recovery yield and salt rejection, a readily adjustable lever that can be particularly beneficial for fit-for-purpose end uses that permit different salinities.^{1,24,25}

Intermediate Step Does Not Introduce Significant Solvent Loss. Solvent loss (*L*), defined as the percentage of initial solvent that has partitioned into the aqueous raffinate and product water phases, is presented for TSSE-IR and c-TSSE in Figure 3A for DIPA and in Figures S3A–B of the Supporting Information for TEA and TOA. Amine contents of the raffinates (R_I and R_{II}) and product water (PW) aqueous phases were characterized and their contributions to overall *L* assessed (dark, medium, and light orange stacked columns, respectively). Critically, the introduction of the intermediate step in TSSE-IR results in little to no additional solvent loss compared with c-TSSE for the three solvents examined.

For all three solvents, total Ls are statistically indistinguishable (p > 0.05, Table S1 of the Supporting Information)between TSSE-IR and c-TSSE with $T_{\rm L}$ = 15 °C. The extraction steps are identical. Therefore, the Ls of R_Is , where the majority of solvent loss occurs, are the same. The volumes of water extracted are also equivalent. Because a sufficiently high $T_{\rm H}$ is utilized, the total volume of water released in the intermediate and final disengagement steps of TSSE-IR is practically equal to the volume of product water in c-TSSE with $T_{\rm L}$ = 15 °C (Figure S4 of the Supporting Information). Summing the individual Ls across the steps, therefore, yields net solvent losses that are effectively similar between the two operations. Despite differences in product water salinities, residual solvent concentrations in the product waters are also similar (Table S1 of the Supporting Information) due to low mutual solubilities at high $T_{\rm H}^{11,26,27}$ These trends hold true for all three solvents studied in this investigation.

Total *Ls* for c-TSSE with $T_{\rm L} = 30$ °C are statistically indistinguishable (p > 0.05, Table S1 of the Supporting Information) from TSSE-IR for DIPA and within a factor of 2 for TEA and TOA. Differences in temperatures as well as salt concentrations and masses of the aqueous phases between



Figure 3. (A) Percentage of solvent loss, L, for 1.0 M NaCl brine feeds and the amine solvent diisopropylamine (DIPA). c-TSSE with $T_{\rm L}$ values of 15 and 30 $^{\circ}{\rm C}$ (left open and right hatched columns, respectively) are compared to TSSE-IR with $T_{\rm L}$ = 15 °C and $T_{\rm IR}$ = 30 °C (center filled columns). All three operations utilize $T_{\rm H}$ = 70 °C. Dark, medium, and light orange stacked columns indicate the contributions, where applicable, from R_I (raffinate from Step I of Figure 1), R_{II} (raffinate from Step II), and PW (product water), respectively. (B) Molar ratio of water to salt in the organic phase, $n_{\rm w}^{\rm org}$: $n_{\rm s}^{\rm org}$, as a function of mole fraction of water in the organic phases, x_w^{org} , for DIPA-H₂O-NaCl mixtures. Circle symbols signify c-TSSE with 1.0 M NaCl initial feed at $T_{\rm L}$ = 15, 20, 25, and 30 °C, and the red square symbol denotes TSSE-IR with $T_{\rm L}$ = 15 °C and $T_{\rm IR}$ = 30 °C. Straight lines connecting the c-TSSE circle symbols are drawn in to serve as visual guides. For all plots in this figure, data and error bars are means and one standard deviation, respectively, from duplicate experiments.

these two operations counterbalanced each other, thus resulting in the observed comparable solvent losses (detailed discussion can be found in the Supporting Information).^{18,20,26,28} Therefore, the improvements in salt rejections of TSSE-IR compared with conventional operation are not at the expense of higher solvent losses.

In practical operations of TSSE, solvent residues in the aqueous phases can be recovered and cycled back to the process.¹⁵ Salt concentrations of the final raffinates can be near the saturation limit, significantly reducing the total L of the process. For example, DIPA loss to a 5.0 M NaCl brine is 0.55

 \pm 0.02% at 15 °C, a 5.0× decrease compared to *L* to R_I in c-TSSE with $T_{\rm L} = 15$ °C. Raising the temperature of the raffinates will further drive the demixing of amines for recovery.^{16,23} At 70 °C, DIPA loss to a 5.0 M NaCl brine is 0.24 \pm 0.01%, i.e., an 11.4× decrease in *L* relative to R_I for c-TSSE with $T_{\rm L} = 15$ °C. TEA leakage is similarly suppressed, whereas TOA loss to the highly concentrated and warmed raffinate is impressively low at 0.0041 \pm 0.0004% (results of solvent loss to highly saturated raffinates and with temperature swing recovery are summarized in Table S2 of the Supporting Information.) Reverse osmosis posttreatment has been demonstrated to remove and recover almost all the solvent in desalinated product waters.¹⁵ Posttreated product waters can be suitable for fit-for-purpose applications, e.g., agricultural reuse.

TSSE-IR Advances the Productivity-Selectivity Tradeoff that Constrains Single-Step Operation. Salt contents of the organic phase, x_s^{org} , are more sensitive to changes in temperature than water contents of the organic phase, x_w^{org} (*x* is mole fraction, superscript org indicates organic phase, and subscripts s and w represent salt and water, respectively). Raising the temperature from 15 to 30 °C depresses x_s^{org} s by an order of magnitude, whereas x_w^{org} s only marginally decline, well within a factor of 1 (liquid–liquid equilibrium phase diagrams of DIPA–H₂O–NaCl systems are presented in Figures S5A– C of the Supporting Information). Increasing the temperature further to 70 °C suppresses x_s^{org} s below detection limits, whereas x_w^{org} s are still within the same order of magnitude.

TSSE-IR advances the productivity-selectivity trade-off by taking advantage of these differences in water and salt partitioning behaviors and leveraging a higher organic:aqueous phase ratio in the intermediate step (as previously discussed). x_{w}^{org} represents the amount of water extracted by the solvent and is thereby related to productivity. The molar ratio of water to salt in the organic phase, n_w^{org} : n_s^{org} , ultimately determines salt rejection performance and, hence, can be a proxy for selectivity. x_{w}^{org} and n_{w}^{org} : n_{s}^{org} are evaluated for c-TSSE (T_{L} = 15–30 °C) and TSSE-IR ($T_{\rm L}$ = 15 °C and $T_{\rm IR}$ = 30 °C) and presented in the productivity-selectivity plot of Figure 3B (detailed method on the analysis using ternary phase diagrams, Figures S5A–C, can be found in the Supporting Information). In c-TSSE, selectivity decreases as productivity increases, as denoted by the negatively sloping trend of the circle symbols.²⁰ Across $T_{\rm L}$ s of 15–30 °C, the interpolated productivity– selectivity observed for c-TSSE falls below TSSE-IR (circle and orange square symbols, respectively). Optimization of the c-TSSE extraction temperature is, therefore, unlikely to produce better performance than TSSE-IR. On the other hand, further engineering of the intermediate step temperature, $T_{\rm IR}$, can improve overall desalination outcome by balancing enhancements in salt rejection with minimized sacrifices in water recovery vield.

TSSE-IR Performance Can Be Determined by Hunter– Nash Analysis of Ternary Diagrams. The Hunter–Nash method can use equilibrium ternary diagrams (Figures S5A–C of the Supporting Information) to predict trends in water recovery yields (Y) and salt rejections (SR) for both TSSE-IR and c-TSSE with good qualitative agreement (Pearson's correlation coefficients ≥ 0.98, Tables S3 and S4 of the Supporting Information). As a result of the differences in water and salt partitioning behavior, the Hunter–Nash analysis modeled SR to improve by 2.8× and Y to change by -42% for TSSE-IR compared to c-TSSE with $T_{\rm L}$ = 15 °C (Tables S3 and S4), i.e., the gain in salt rejection significantly outweighs the diminished water recovery yield. Due to the dramatic decrease in x_s^{org} at 30 °C, modeled *SRs* are approximately equivalent at >90% for both c-TSSE with $T_L = 30$ °C and TSSE-IR, matching experimental observations (Table S4). Because the solvent is able to retain more water in TSSE-IR compared to c-TSSE with $T_L = 30$ °C (as discussed above), the water recovery yield modeled by the Hunter–Nash analysis is correspondingly 115% larger for TSSE-IR (Table S3). Further details on the analysis method can be found in the Supporting Information.

Implications of TSSE-IR for Hypersaline Brine Desalination. This study demonstrates improved performance of the novel temperature swing solvent extraction with intermediate-step release for the desalination of hypersaline brines over the conventional single-step TSSE. By taking advantage of differences in water and salt partitioning behaviors, TSSE-IR advances the productivity-selectivity trade-off of conventional TSSE. Fine-tuned selection of the intermediate temperature can enable further optimization between water recovery yield and salt rejection, and product water quality can be calibrated for specific performance objectives, e.g., fit-for-purpose applications that permit TDS concentrations above drinking water standards and low concentrations of residual solvents. Process waters for oil and gas extraction, mining, textiles, leather tanning, pulp and paper, and certain chemical manufacturing operations may be well-suited for reuse applications. As the majority of extracted salt disengages from the water-in-solvent extract during the intermediate step, additional intermediate steps are likely to offer only marginal improvement in salt rejection at the expense of further reducing the water recovery yield.

TSSE-IR enables dramatic improvements in salt rejection with minimal sacrifices in water recovery yield and can thereby significantly widen the operable temperature range of the switchable solvents. For example, DIPA and TOA have low salt rejections (<50%) at the extraction temperature of 15 °C, which renders them unsuitable for conventional TSSE. However, with the intermediate release step, the two solvents can achieve adequately high salt rejections while exploiting the enhanced water extractions at 15 °C. Performance trends are not solvent-specific and can be generally extended to different solvent classes, e.g., organic acids, ionic liquids, and polyethers. Hence, this approach can be used to expand the spectrum of viable solvents for hypersaline desalination to include safer and more environmentally sustainable chemicals that exhibit high water productivity but low selectivity in single-stage TSSE operations. The use of more benign solvents would further broaden fit-for-purpose reuse opportunities to include applications such as cooling tower makeup and dust control. Other solvents may experience less loss to the aqueous phases, a strategic research aim for practical implementation of solvent extraction desalination.²

ASSOCIATED CONTENT

S Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.estlett.3c00616.

Detailed descriptions of materials and chemicals, compositional characterization of biphasic mixtures, and Hunter–Nash and statistical analysis methodologies (PDF)

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Notes

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