*Supporting information for*:

# Optimization across water-energy nexus for integrating heat, power and water for industrial processes coupled with hybrid thermal-membrane desalination

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## Steam and water properties

The steam and water properties were estimated via correlations developed by Al-Azri et al. [1] with some modifications for this study. These equations are shown in Table S1.

**Table S1** Correlations for steam and water thermodynamic properties

| Equation | Description |
|---|---|
| $T_{sat} = 117.66 P_{sat}^{0.2219}$ | Saturation temperature [a]<br>($14.7 \leq P_{sat} \leq 2400$ psia)<br>Error $= \pm 0.79\%$ |
| $T_{sat} = 102.80 P_{sat}^{0.2741}$ | Saturation temperature [a]<br>($1.5 \leq P_{sat} \leq 14.7$ psia)<br>Error $= \pm 1.76\%$ |
| $s_{sat}^{f} = 1.6308 \times 10^{-3} T_{sat} - 3.0838 \times 10^{-2}$ | Saturated water entropy [a]<br>($1.5 \leq P_{sat} \leq 14.7$ psia)<br>Error $= \pm 0.87\%$ |
| $s_{sat}^{v} = -3.9857 \times 10^{-9} T_{sat}^{3} + 5.4089 \times 10^{-6} T_{sat}^{2} - 3.3698 \times 10^{-3} T_{sat} + 2.2658$ | Saturated steam entropy [a]<br>($1.5 \leq P_{sat} \leq 2400$ psia)<br>Error $= \pm 0.37\%$ |
| $s^{v} = s_{sat}^{v} + 0.46883 - 0.46883 \exp\left(-k_{T} \Delta T_{sat}\right)$<br><br>$k_{T} = 1.3845 \times 10^{-2} \left(\dfrac{T_{sat}}{1000}\right)^{2} - 9.8258 \times 10^{-3} \left(\dfrac{T_{sat}}{1000}\right) + 3.1462 \times 10^{-3}$<br><br>$\Delta T_{sat} = T - T_{sat}$ | Entropy of steam [a]<br>$14.7$ psia $< P < 1500$ psia<br>$T_{sat} \leq T \leq 1300$ °F<br>Error $= \pm 1.36\%$ |
| $H_{sat}^{f} = 4.2433 \times 10^{-5} T_{sat}^{2} + 9.8773 T_{sat} - 31.146$ | Saturated water enthalpy [a]<br>$1.5$ psia $< P_{sat} < 14.7$ psia<br>Error $= \pm 0.02\%$ |

[a] This study; [b] Adopted from work by Al-Azri et al. [1]

**Table S1** Correlations for steam and water thermodynamic properties*(Continued)*

| Equations | Descriptions |
|---|---|
| $H_{sat}^{f} = 4.5395 \times 10^{-4} T_{sat}^{2} + 0.74207 T_{sat} + 4.8112$ | Saturated water enthalpy [a] <br> $14.7 \text{ psia} < P_{sat} < 1500 \text{ psia}$ <br> Error $= \pm 1.26\%$ |
| $H_{sat}^{v} = -2.0449 \times 10^{-4} T_{sat}^{2} + 0.47202 T_{sat} + 1.0595$ | Saturated steam enthalpy [a] <br> $1.5 \text{ psia} < P_{sat} < 14.7 \text{ psia}$ <br> Error $= \pm 0.01\%$ |
| $H^{v} = 0.2029 T_{sat} \left(s^{v}\right)^{3.647} + 817.35$ | Enthalpy steam [b] <br> Error $= \pm 0.66\%$ |

## Turbine modeling

**Table S2** Regression coefficients used in isentropic efficiency equation

| Coefficient | Back Pressure turbines | | Condensing turbines | |
|---|---|---|---|---|
| | $W^{max}$ <br> $< 4.1 \text{MMBtu/hr}$ | $W^{max}$ <br> $> 4.1 \text{ MMBtu/hr}$ | $W^{max}$ <br> $< 5.12 \text{ MMBtu/hr}$ | $W^{max}$ <br> $> 5.12 \text{ MMBtu/hr}$ |
| $a_{o}$ [Btu/hr] | -0.1508 | -1.038755556 | -0.115877778 | -0.062488889 |
| $a_{1}$ [Btu/hr-°F] | 0.00065 | 0.003461111 | 0.000555556 | 0.000777778 |
| $b_{o}$ [Btu/hr] | 0.961977778 | 1.111644444 | 1.195233333 | 1.166466667 |
| $b_{1}$ [Btu/hr-°F] | 0.000844444 | 0.000261111 | 0.000333333 | 0.000166667 |

The coefficients are taken from Varbanov et al. [2] and Mavromatis and Kokosiss [3] with original values expressed in SI units.

## MED process modeling

The general mass and salt component balance equations for all effects, the down condenser and the distillate flashing boxes are given by Equations 50 - 55 and are summarized in

**Table S3**. In addition, the corresponding energy balances are given by Equations 56 - 64 for all the effects as well as the condenser, distillate flashing boxes and steam ejector. These energy balances are described in more detail by Gabriel et al. [4]. They represent an alternative approach to modeling the MED-TVC process from the previously utilized specific heat capacity model.

**Table S3** Mass and energy balance equations for MED-TVC process

| Equations | Descriptions |
|---|---|
| $F^{MED} = \sum\limits_{i \in N_{eff}} F_i^{MED}$ | Total MED feed flow |
| $F_i^{MED} = V_i + B_i$ | Mass balance on effect 1 |
| $F_i^{MED} + B_{i-1} = V_i + B_i$ | Mass balance on effect 2 to $N_{eff}$ |
| $M_{sea}^{cond} = \dfrac{\left(V_N + M_{pot,N_{eff}-1}^{stm} - Dr\right) \cdot \lambda_{cond}}{Cp \cdot \left(T_f - T_{sea}^{IN}\right)}$ | Cooling seawater balance on condenser |
| $M_{feed}^{salt} = M_1^{salt}$ | Salt balance on effect 1 |
| $M_{feed}^{salt} + M_{i-1}^{salt} = M_i^{salt}$ | Salt balance on effect 2 to $N_{eff}$ |
| $Q_i^{EVAP} + M_{feed} H_{feed} + \dfrac{Q^{PRE}}{N_{eff}} = M_{feed,i}^{stm} H_i^v + M_{feed,i}^{brine} H_i^{brine}$ | Energy balance on effect evaporator |
| $Q_i^{EVAP} = Q_i^{vap} + Q_i^{sens}$ $Q_i^{vap} = M_{feed,i}^{stm} H_i^v$ | Energy distribution of effect evaporator |
| $M_{feed,i-1}^{brine} H_{feed,i-1}^{brine} + M_{BF,i-1}^{brine} H_{BF,i-1}^{brine} = M_{BF,i}^{brine} H_{BF,i}^{brine}$ $+ M_{BF,i}^{stm} H_i^{v'}$ | Energy balance on brine flashing (BF) |
| $M_{brine}^{MED} = M_{BF,N_{eff}}^{brine}$ | MED brine flow |
| $D_{i-1} H_{i-1}^{f''} + M_i^c H_{i-1}^c = M_{pot,i}^{stm} H_i^{v''} + M_{pot,i}^{water} H_i^{f''}$ | Distillate (D) flashing pot balance |
| $M_{pot,i}^{water} = M_{DS,i}^{water} + M_{BFW,i} + D_i$ | Mass balance on flash pot outflow (W) |
| $M_{perm}^{MED} = D_{N-1} + \left(V_{N_{eff}} + M_{pot,N_{eff}-1}^{stm}\right) - Dr$ | MED permeate flow |
| $S_{mot} \cdot H_{mot}^v + Dr \cdot H_{N_{eff}}^v + \sum\limits_{i=1}^{N} M_{DS,i}^{water} H_i^{f''} = M_{DS}^{stm} H_{DS}^v$ $+ M_{DS}^c H_{DS}^f$ | De-superheater balance |

## Heat transfer area calculations

The heat transfer coefficient, logarithmic mean temperature difference and corresponding area for each effect is calculated using equations given in Table S4.

**Table S4** Equations for calculating the heat transfer area, logarithmic mean temperature difference and overall heat transfer coefficients for MED-TVC process

| Equations | Descriptions |
|---|---|
| $$A_i^{vap} = \frac{Q_i^{vap}}{U_i^{eff}\left(T_{i-1}^c - T_i^{eff}\right)}$$ | Vaporization heat transfer area for each evaporator |
| $$A_i^{sens} = \frac{Q_i^{sens}}{U_i^{eff}\left(LMTD\right)_i^{sens}}$$ | Sensible heat transfer area for each evaporator |
| $$A_i^{Total} = A_i^{vap} + A_i^{sens}$$ | Total heat transfer area for each evaporator |
| $$A_{cond} = \frac{Q_{total}^{COND}}{U_{cond}\left(LMTD\right)_{cond}}$$ | Condenser heat transfer area |
| $$\left(LMTD\right)_i^{sens} = \left[\left(T_{i-1}^c - T_f\right)\cdot\left(T_{i-1}^c - T_i^{eff}\right)\cdot\left(T_{i-1}^c - \frac{T_f + T_i^{eff}}{2}\right)\right]^{\frac{1}{3}}$$ | Logarithmic mean temperature difference for each effect based on approximation by Chen et al. [5] |
| $$\left(LMTD\right)_{cond} = \left[\left(T_{N_{eff}}^c - T_f\right)\cdot\left(T_{N_{eff}}^c - T_{sea}^{IN}\right)\cdot\left(T_{N_{eff}}^c - \frac{T_f + T_{sea}^{IN}}{2}\right)\right]^{\frac{1}{3}}$$ | Logarithmic mean temperature difference for condenser based on approximation by Chen at al. [5] |
| $$U_i^{eff} = 2.318\times10^{-6}\left(T_i^{eff}\right)^3 - 2.0752\times10^{-4}\left(T_i^{eff}\right)^2 + 1.4056\times10^{-3}\left(T_i^{eff}\right) + 1.9394$$ | Overall heat transfer coefficient for evaporator |
| $$U_{cond} = -8.026\times10^{-8}\left(T_{N_{eff}}^c\right)^3 + 1.825\times10^{-4}\left(T_N^c\right)^2 + 1.537\times10^{-4}\left(T_{N_{eff}}^c\right) + 1.6175$$ | Overall heat transfer coefficient for condenser |

Overall heat transfer coefficients for evaporator and condenser are presented in their original units as described in work by El-Dessouky et al. [6]

**Effect temperature profile**

The temperature profile of the saturated vapor, condensate, brine and distillate are calculated using the equations given in Table S5.

**Table S5** Equations for calculating the temperature profile of saturated vaporheat transfer area, logarithmic mean temperature difference and overall heat transfer coefficients for MED-TVC process

| Equations | Description |
|---|---|
| $\Delta T^{eff} = \dfrac{T_1^{eff} - T_N^{eff}}{N_{eff} - 1}$ | Temperature difference of all effects |
| $T^{DS} = T_1^{eff} + \Delta T^{eff}$ | Temperature of steam from de-superheater |
| $T_{i+1}^{eff} = T_i^{eff} - \Delta T^{eff}$ | Temperature of effects 2 to $N_{eff}$ |
| $T_f \leq T_N^c - \Delta T_{min}^{cond}$ | Feed seawater temperature constraint |
| $T_i^v = T_i^{eff} - BPE_i$ | Temperature of vapor formed in each effect |
| $T_i^{brine} = T_i^{eff} + NEA_i^{brine}$ | Temperature of flashed brine |
| $T_i^{flash} = T_i^v + NEA_i^{flash}$ | Temperature of flashed distillate |
| $BPE = C\left(X_{sal}^{eff}\right)^2 + D\left(X_{sal}^{eff}\right)$ <br> $C = -4.584 \times 10^{-4}\left(T^{eff}\right)^2 + 0.2823\left(T^{eff}\right) + 17.95$ <br> $D = 1.536 \times 10^{-4}\left(T^{eff}\right)^2 + 5.267 \times 10^{-2}\left(T^{eff}\right) + 6.56$ | Boiling point elevation [7]. |
| $NEA_i^{brine} = \dfrac{33 \cdot \left(T_{i-1}^{eff} - T_i^{eff}\right)^{0.55}}{T_i^v}$ | Non-equilibrium allowance for flashing brine |
| $NEA_i^{flash} = \dfrac{0.33 \cdot \left(T_{i-1}^c - T_i^v\right)}{T_i^v}$ | Non-equilibrium allowance for flashing distillate |

**Reverse Osmosis (RO) unit modeling**

Design and operating parameters used in RO network optimization are given in Table S6. The RO unit was modeled using correlations developed by DOW and utilized in their Reverse Osmosis Systems Analysis (ROSA) Filmtec software [8]. These equations are given in Table S7 along with the mass balances for the RO units.

**Table S6** Design and operating parameters for Reverse osmosis network (RON)

| Parameter | Unit | Value |
|---|---|---|
| Final permeate pressure | psia | 14.5 |
| Final reject pressure | psia | 14.5 |
| Energy recovery device efficiency | % | 80 |
| Pump efficiency | % | 80 |
| Seawater feed temperature | °F | 77 |
| Maximum pressure drop across RO unit | psia | 18.9 |
| Maximum feed pressure to RO unit | psia | 1015 |
| Maximum number of modules in one unit | | 1000 |
| Membrane area per module (6 elements/module) | ft$^2$ | 2641 |

**Table S7** General modeling equations for reverse osmosis (RO) unit

| Equations | Descriptions |
|---|---|
| $$NM = \dfrac{M^{RO}_{feed}}{SM \cdot \overline{A}(\overline{\pi}) \cdot TCF \cdot FF \cdot \rho_f \cdot \left[ P_f - \dfrac{\overline{\Delta P}_{fc}}{2} - P_p - \pi_{pf} \right]}$$ | Number of modules |
| $$\pi_{pf} = \pi_f \left( \dfrac{\overline{C}_{fc}}{C_f} pf + \overline{R} - 1 \right)$$ | |
| if $\pi_f \leq 2$ $\quad \overline{A}(\overline{\pi}) = 0.125$ | Membrane permeability at 25°C |
| if $25 \leq \pi_f \leq 200$ $\quad \overline{A}(\overline{\pi}) = 0.125 - 0.011 \cdot \left( \dfrac{\pi_f - 25}{35} \right)$ | |
| if $200 \leq \pi_f \leq 400$ $\quad \overline{A}(\overline{\pi}) = 0.070 - 0.0001 \cdot (\pi_f - 200)$ | |
| if $T \geq 25$, $\quad TCF = \exp\left[ 2640 \cdot \left( \dfrac{1}{298} - \dfrac{1}{273+T} \right) \right]$ | Temperature correction factor |
| if $T \leq 25$, $\quad TCF = \exp\left[ 3020 \cdot \left( \dfrac{1}{298} - \dfrac{1}{273+T} \right) \right]$ | |
| $$\overline{\Delta P}_{fc} = 0.04 \cdot \left( \dfrac{M^{RO}_{feed} + M^{RO}_{brine}}{2 \cdot NM \cdot \overline{\rho}} \right)^2$$ | Average concentrate side system pressure drop |
| $$\dfrac{\overline{C}_{fc}}{C_f} = -\dfrac{\ln(1-Y)}{Y}$$ | Approximate log-mean concentrates side to feed concentration ratio for system |
| $$\pi_{feed} = 1.12 \cdot (273+T) \cdot \sum_{i=1}^{Nc} m_i \qquad i \in Nc$$ | Feed osmotic pressure |
| $$pf = \exp(0.7Y)$$ | Concentration polarization factor |

| | |
|---|---|
| $F^{RO} = M_{perm}^{RO} + M_{brine}^{RO}$ | Mass balance on RO unit |
| $X_{feed}^{RO} F^{RO} = X_{perm}^{RO} M_{perm}^{RO} + X_{brine}^{RO} M_{brine}^{RO}$<br>$X_{feed}^{RO} = \sum_{i \in Nc} X_{feed,i}^{RO}$<br>$X_{perm}^{RO} = \sum_{i \in Nc} X_{perm,i}^{RO}$<br>$X_{brine}^{RO} = \sum_{i \in Nc} X_{brine,i}^{RO} \qquad i \in Nc$ | Salt balance on RO unit |
| $Y = \dfrac{M_{perm}^{RO}}{F^{RO}}$ | RO unit recovery |
| $\overline{R} = 1 - \dfrac{X_{perm}^{RO}}{X_{feed}^{RO}}$ | Average salt rejection |

The coefficients used to determine air cooling and cooling water tower power consumption rates are given in Table S8. In addition, cooling tower makeup water requirements based on evaporative losses is also calculated using coefficients given in Table S8. These parameters were adopted from previous studies [9].

**Table S8** Cooling utility power and water requirement factors

| Cooling parameter | Value |
|---|---|
| Air cooler draft fan power     [kW/MMBtu/hr] | 1.000 |
| Cooling tower daft fan power [kW/MMBtu/hr] | 0.092 |
| Cooling tower water makeup    [lb/MMBtu/hr] | 1.000 |

## NOMENCLATURE

| | |
|---|---|
| $A_i$ | Heat transfer area in $i$th effect |
| $A_{ij}$ | Area for heat transfer between $i$th HPS and $j$th US |
| $\overline{A}(\overline{\pi})$ | Membrane permeability |
| $B_i$ | Brine flow from $i$th effect |
| $BPE$ | Boiling point elevation |
| $Cp$ | Specific heat capacity |
| $\dfrac{\overline{C}_{fc}}{C_f}$ | Log mean concentrate-side to feed concentration ratio in RO unit |

| | |
|---|---|
| $D_i$ | Distillate mass flowrate from $i$th flash pot |
| $Dr$ | Mass flowrate of entrained steam from final effect |
| $F$ | Flowrate |
| $FF$ | Fouling factor of RO unit |
| $H$ | Enthalpy of stream |
| $LMTD$ | Logarithmic mean temperature difference |
| $\dot{m}$ | Mass flowrate of stream |
| $M$ | Mass flowrate of stream |
| $N$ | Number of effects |
| $NEA$ | Non-equilibrium allowance |
| $NM$ | Number of modules |
| $pf$ | Concentration polarization factor |
| $P_f$ | Feed pressure to RO unit |
| $P_p$ | Permeate pressure from RO unit |
| $\overline{\Delta P}_{fc}$ | Average concentrate-side system pressure drop for RO unit |
| $Q$ | Heat exchanger duty |
| $\overline{R}$ | Average salt rejection of RO unit |
| $S$ | Steam mass flowrate |
| $SM$ | Module surface area of RO unit |
| $SUMDT_{i,j}$ | Sum of heat exchanger temperature differences |
| $T$ | Temperature |
| $TCF$ | Temperature correction factor or RO unit |
| $\Delta T$ | Temperature difference |
| $U$ | Heat transfer coefficient of heat exchanger |
| $V_i$ | Vapor flow from $i$th effect |
| $X$ | Salt concentration in feed to RO unit |
| $Y$ | Recovery of RO unit |

**Greek letters**

| | |
|---|---|
| $\eta$ | Unit efficiency |

| | |
|---|---|
| $\lambda$ | Latent heat of vaporization |
| $\pi_f$ | Osmotic pressure of seawater feed to RO unit |
| $\rho$ | Density of fluid |

**Defined sets**

| | |
|---|---|
| *Nc* | Number of components |

**Subscripts and superscripts**

| | |
|---|---|
| *a* | Actual exit conditions |
| *BF* | Brine flashing |
| *BFW* | Boiler feed water stream |
| *c* | Condensate stream |
| *cond* | Condenser |
| *DS* | De-superheater |
| *EX* | Exit conditions |
| *exh* | Exhaust conditions |
| *f* | Saturated water conditions |
| *f'* | Saturated water conditions in brine flashing |
| *f"* | Saturated water conditions in distillate flashing |
| *MED* | Multi-effect distillation unit |
| *mot* | Motive |
| *RO* | Reverse osmosis unit |
| *s* | Salt |
| *s'* | Salt in brine flashing |
| *v* | Vapor conditions |
| *v'* | Vapor conditions in brine flashing |
| *v"* | Vapor conditions in distillate flashing |
| *vac* | Vacuum conditions |

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