

1 Thermo-Economic and Environmental Optimization of a 2 Solar-based Zero-Liquid Discharge System for Shale Gas 3 Wastewater Desalination

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1 **ABSTRACT**

2 Wastewater management is one of the main hurdles encountered by the shale
3 gas industry for boosting overall process cost-effectiveness while reducing
4 environmental impacts. In this light, we introduce a new multi-objective model
5 for the thermo-economic and environmental optimization of solar-based zero-
6 liquid discharge (ZLD) desalination systems. The solar-driven ZLD system is
7 specially developed for the desalination of high-salinity shale gas wastewaters. A
8 decentralized system is proposed, which encompasses a solar thermal system
9 (STS), a Rankine cycle unit, and a multiple-effect evaporation with mechanical
10 vapor recompression (MEE-MVR) plant. The environment-friendly ZLD operation
11 is ensured by specifying the discharge brine salinity close to salt saturation
12 conditions. The mathematical model is formulated as a multi-objective non-linear
13 programming (NLP) problem, aimed at the simultaneous minimization of thermo-
14 economic and environmental objective functions. The latter objective function is
15 quantified by the life cycle assessment (LCA)-based ReCiPe methodology. The
16 multi-objective NLP model is implemented in GAMS software, and solved through
17 the epsilon-constraint method. A set of trade-off Pareto-optimal solutions is
18 presented to support decision-makers towards implementing more sustainable
19 and cost-efficient solar-driven ZLD desalination systems. Our comprehensive
20 energy, economic and environmental analysis reveals that the innovative system
21 can significantly decrease costs and environmental impacts in shale gas
22 wastewater operations.

23

24 **Keywords:** Optimization, shale gas wastewater, high-salinity wastewater, zero-
25 liquid discharge (ZLD), multiple-effect evaporation (MEE), mechanical vapor
26 recompression (MVR), renewable energy.

1 **1. Introduction**

2 Advances in horizontal drilling and hydraulic fracturing technologies allied to
3 supportive policies have fueled large-scale shale gas exploration worldwide
4 throughout the last decade. Notwithstanding, the intensification in shale gas
5 production around the world has also fostered concerns about adverse effects on
6 communities, public health and the environment. The environmental impacts are
7 mainly associated with induced seismic events (NRC, 2013), greenhouse gas
8 (GHG) emissions (Staddon and Depledge, 2015), and depletion of water resources
9 and wastewater pollution (Prpich et al., 2016; Thomas et al., 2017). Regarding the
10 water-related implications, the gas extraction process from shale reservoirs
11 usually requires significant volumes of water and generates excessive amounts of
12 high-salinity wastewater (Onishi et al., 2019). As a result, wastewater management
13 is one of the main obstacles faced by the shale gas industry to improve overall
14 cost-effectiveness and reduce environmental impacts (Kausley et al., 2017; Onishi
15 et al., 2018).

16 In shale gas operations, thermal desalination systems based on multiple-
17 effect evaporation with mechanical vapor recompression (MEE-MVR) provide a
18 viable solution for the zero-liquid discharge (ZLD) treatment of high-salinity
19 wastewaters from gas extraction. Onishi et al. (2017b) have developed a non-
20 linear programming (NLP) model for the systematic optimization of ZLD
21 desalination processes. The authors have carried out a thorough comparison of
22 several system configurations –single/multiple-effect evaporation (SEE/MEE)
23 with/without multistage compression and thermal integration– in terms of
24 producing freshwater and achieving ZLD conditions under different inlet
25 conditions. Their comprehensive energy and economic analysis have shown that
26 the MEE-MVR system is the most cost-effective process for the ZLD desalination
27 of shale gas wastewater. The authors have estimated treatment costs ranging
28 from 6.7–10.9 US\$/m³ depending on the system configuration, while disposal

1 costs in conventional Class II saline water injection wells are projected to be
2 between 8–25 US\$/m³ (Acharya et al., 2011; Onishi et al., 2018). In Onishi et al.
3 (2017a), the authors have extended their previous modelling approach to allow
4 for the estimation of the most relevant geometrical characteristics of the
5 desalination system during the optimization task. Their improved rigorous model
6 has also highlighted the potential of ZLD desalination for the effective and
7 economic shale gas wastewater treatment.

8 For addressing the uncertainty associated with shale gas wastewater data,
9 Onishi et al. (2017c) have introduced a stochastic multiscenario NLP-based model
10 for the optimal design of ZLD desalination systems. In this approach, the authors
11 have considered both wastewater salinity and flowrate as uncertain design
12 parameters to enhance system flexibility and reliability. Thus, the latter uncertain
13 parameters have been modelled as a set of correlated feeding water scenarios
14 with a given probability of occurrence. The authors have presented cumulative
15 probability curves to appraise the economic risk linked to the uncertain space for
16 distinct standard deviations of expected mean values. Their results reveal that the
17 proposed stochastic multiscenario approach leads to improved thermo-economic
18 performance solutions in comparison to previous deterministic models.

19 Although aforementioned studies have highlighted the feasibility of zero-
20 liquid discharge MEE-MVR desalination systems for reducing wastewater impacts
21 while improving water resources, their practical implementation is still restricted
22 by their intensive energy consumption and associated pollutant carbon
23 emissions. For instance, the SEE/MEE-MVR technologies for ZLD desalination
24 developed in Onishi et al. (2017b) have presented specific energy consumption
25 ranging from 28–50.5 kWh_e per cubic meter of produced freshwater. According
26 to the US Energy Information Administration (EIA, 2016), about 939 g/kWh_e of
27 CO₂ are generated to produce electricity from burning coal. Under the latter
28 assumption, the referred SEE/MEE-MVR systems operating at ZLD conditions
29 would yield to ~26–47 kg of CO₂ per cubic meter of produced freshwater (Onishi

1 et al., 2018; Onishi et al., 2017b). These results emphasize the need for developing
2 more sustainable alternatives for ZLD desalination systems, particularly involving
3 the integration of renewable energy resources.

4 The integration of solar thermal energy to power desalination systems has
5 attracted increased interest from the literature over the past few years. Into this
6 framework, Pouyfaucou and García-Rodríguez (2018) have studied different solar
7 thermal-powered desalination technologies to identify main issues for improving
8 market opportunities. The authors have presented a thorough performance and
9 economic analysis of distinct membrane distillation (MD) and reverse osmosis
10 (RO)-based desalination systems assisted by solar photovoltaic and solar thermal
11 power plants. Their analysis has included parabolic trough collectors, linear
12 Fresnel concentrators, and dish concentrators. Moore et al. (2018) have examined
13 the coupling of thermal solar thermal collectors to sweeping-gas MD systems via
14 economic optimization. Karanikola et al. (2019) have also provided an economic
15 performance evaluation of MD desalination system driven by solar photovoltaic
16 and solar thermal collectors. Zheng and Hatzell (2020) have developed a techno-
17 economic model to evaluate the viability of combining solar collectors with
18 multistage flash distillation (MSF) systems. Their model accounts for several
19 factors such as system lifetime and scale, performance parameters of different
20 system units, and payback period, aimed at surpassing geographic and technical
21 constraints.

22 Aboelmaaref et al. (2020) have presented a comprehensive review on
23 concentrated solar power (CSP) desalination technologies. The authors have paid
24 particular attention on the thermodynamic and economic analysis of desalination
25 systems driven by parabolic trough collectors and parabolic dish CSP
26 technologies. Ghenai et al. (2021) have proposed an optimization approach based
27 on response surface for improving hybrid multi-effect distillation (MED) and
28 adsorption desalination (AD) systems powered by solar thermal energy. Their
29 optimization method, along with performance analysis and parametric study, are

1 used to identify the optimal operating conditions to increase the freshwater
2 production while reducing energy consumption. Even though previous studies
3 have presented insightful results on the integration of solar thermal technologies
4 to desalination plants, none of them have considered ZLD processes. To tackle
5 this issue, Najaf et al. (2019) have performed a thermo-economic evaluation of a
6 ZLD desalination plant equipped with parabolic trough solar collectors. Their
7 simulation model approach is focused on an industrial wastewater treatment
8 plant composed of a brine concentrator and a forced-circulation crystallizer.
9 However, their approach disregards energy intensive high-salinity applications, as
10 well as the assessment of environmental impacts of the process.

11 To overcome shortcomings in preceding research, we introduce a new
12 multi-objective modelling approach for the thermo-economic and environmental
13 optimization of solar-driven ZLD desalination systems. The mathematical model
14 is developed upon a multistage superstructure, which includes a solar thermal
15 system (STS), a Rankine cycle (RC) unit, and a MEE-MVR desalination plant. The
16 proposed desalination process is particularly applied for treating high-salinity
17 shale gas wastewaters. In this system, the ZLD operation is ensured by a design
18 constraint that specifies the discharge brine salinity close to salt saturation
19 conditions. Also, the STS is designed to operate in different time periods to
20 account for the intermittency in daily solar irradiance throughout the year. The
21 model is formulated as a multi-objective NLP problem, which is implemented in
22 GAMS software and solved via the epsilon-constraint method to minimize both
23 thermo-economic and environmental objective functions. The environmental
24 performance is evaluated by the LCA-based ReCiPe methodology. Our
25 methodology allows obtaining a set of alternative Pareto-optimal solutions to
26 support decision-makers towards the implementation of more environment-
27 friendly and cost-effective solar-driven ZLD desalination systems.

28 The rest of this paper is organized as follows. In **Section 2**, we briefly
29 introduce the problem statement of multi-objective optimization of solar-driven

1 ZLD desalination systems. The process description of the MEE-MVR desalination
2 plant, and RC and STS units are presented in **Section 3**. In **Section 4**, we
3 developed the multi-objective modelling approach. The illustrative case study
4 used to assess the applicability of the proposed model is described in **Section 5**,
5 while the main results obtained are discussed in **Section 6**. Finally, we summarize
6 the main conclusions in **Section 7**.

7

8 **2. Problem Statement**

9 The multi-objective optimization problem can be formally stated as follows. We
10 are given the inlet feed water (*i.e.*, high-salinity shale gas wastewater) conditions
11 (which include temperature, salinity, and mass flowrate), and the ZLD target state.
12 The technical characteristics of the MEE-MVR system, Rankine cycle units, and
13 solar parabolic trough collectors are also known, along with weather conditions,
14 economic, and environmental impact data. Utilities (electricity, natural gas, and
15 cooling water) are provided with their corresponding prices and environmental
16 data. The main goal is to obtain an optimal design and operating conditions for
17 the solar-based ZLD desalination system that simultaneously enhance its thermal-
18 economic and environmental performances. To do so, a multi-objective NLP-
19 based model is developed and solved via the epsilon-constraint method, through
20 the minimization of the economic and environmental objective functions. In this
21 approach, the solar thermal system (STS) should follow a multi-period operation
22 to account for the different weather conditions throughout the year. In addition,
23 the ZLD operation is ensured by adding a design constraint that sets the
24 discharge salinity close to the salt saturation condition. The process description
25 is presented as follows.

26

27

28

1 **3. Process Description**

2 For our analysis, we consider an integrated system composed of a MEE-MVR
3 desalination plant, STS, and Rankine cycle unit. The schematic diagram for the
4 solar-based ZLD desalination system is displayed in **Fig. 1**.

5 6 **3.1. MEE-MVR Desalination System**

7 The zero-discharge MEE-MVR desalination plant encompasses a multiple-effect
8 horizontal-tube evaporator, which is coupled to intermediate flashing tanks for
9 enhancing energy recovery efficiency. In the system, a feeding-distillate preheater
10 is also used to further increase the thermal integration, whilst the vapor produced
11 by flashing and evaporation processes are managed by a mechanical compressor.
12 Further details on the design and operation of MEE-MVR desalination systems
13 are presented in our previous studies (Onishi et al., 2017a, 2017b, 2017c).

14

15 **3.2. Rankine Cycle Unit**

16 The Rankine cycle unit embraces a steam turbine, a condenser, a pump, and a
17 boiler. The Rankine cycle unit is used to convert the solar energy from the STS
18 into the electric power required by the mechanical vapor compressor in the MEE-
19 MVR desalination plant. In this cycle, the subcooled water (RC working fluid)
20 exchanges heat with the thermal solar fluid of the STS in the boiler to produce
21 superheated vapor. Then, the superheated vapor is used to produce electricity by
22 passing through the turbine generator. The humid vapor from the turbine
23 exchanges heat with cooling water in the condenser before being pumped back
24 to the boiler to restart the cycle.

25

26 **3.3. Solar Thermal System**

27 The STS is comprised by a solar field of parabolic trough collectors, in which the
28 solar thermal energy is transferred to the thermal operating fluid (*i.e.*, mineral oil).

1 A backup natural gas-fired heater (GFH) is used to meet the energy shortages
2 that could result from the daily solar intermittency. The GFH ensures the constant
3 energy supply to the MEE-MVR desalination plant, by keeping the thermal
4 operating fluid of the STS at constant temperature.

5

6 **4. Multi-objective Optimization Model**

7 The multi-objective mathematical model for the optimal design and operation of
8 solar-driven ZLD thermal desalination systems is developed through an NLP-
9 based formulation. The optimization approach encompasses the thermodynamic
10 modelling equations of the MEE-MVR desalination plant, steam Rankine cycle,
11 solar thermal collectors' system, and economic and environmental objective
12 functions. The model is built upon the general superstructure as shown in **Fig. 1**.
13 The multi-objective optimization model is presented in the following sections, in
14 which the solar-driven MEE-MVR superstructure is generated according to the
15 subsequent steps.

16

17 ***4.1. Modelling of the Thermal Desalination System***

18 The mathematical programming model for optimizing the MEE-MVR desalination
19 plant comprises energy and mass balances, temperature and pressure feasibility
20 restrictions, along with the ZLD design constraint. The mathematical formulation
21 is based on our previous studies concerning the design and optimization of MEE-
22 MVR desalination systems presented in Onishi et al. (2017a, 2017b, 2017c). In this
23 study, we take into consideration the following assumptions to simplify the model
24 formulation:

25

- 26 (i) Steady-state operation.
- 27 (ii) Thermal losses in system units are negligible.
- 28 (iii) Vapor streams in evaporator effects are modelled as an ideal gas.

- 1 (iv) Pressure drops in system units are negligible.
 2 (v) The non-equilibrium allowance (NEA) is negligible.
 3 (vi) The mechanical compressor is isentropic.
 4 (vii) The starter power of the mechanical compressor is negligible.
 5 (viii) Capital costs of mixers are negligible.

6

7 The following index set is required for better developing of the NLP-based
 8 model:

$$9 \quad I = \{i / i = 1, 2, \dots, I \text{ is an evaporator effect}\}$$

10

11 4.1.1. Multiple-effect Evaporator Unit

12 The mass balances in the evaporator effect i can be expressed as follows.

13

$$14 \quad \begin{cases} \dot{m}_{i+1}^{brine} = \dot{m}_i^{vapor} + \dot{m}_i^{brine} \\ \dot{m}_i^{brine} \cdot S_i^{brine} = \dot{m}_{i+1}^{brine} \cdot S_{i+1}^{brine} \end{cases} \quad \forall 1 \leq i \leq I-1 \quad (1)$$

$$15 \quad \begin{cases} \dot{m}_i^{feed} = \dot{m}_i^{vapor} + \dot{m}_i^{brine} \\ \dot{m}_i^{feed} \cdot S_{in}^{feed_water} = \dot{m}_i^{brine} \cdot S_i^{brine} \end{cases} \quad \forall i = I \quad (2)$$

16

17 It should be noted that the system operates under a backward feeding
 18 configuration. As a result, the brine salinity in the first evaporation effect $i = 1$
 19 should match the ZLD design constraint (to ensure the ZLD operation), while
 20 salinity of the feed water is considered in the last effect $i = I$. For evaporation
 21 effects in between, that is $1 < i \leq I - 1$, brine is added as feeding stream.

22 The global energy balances in evaporator effects $i \in I$ are given by **Eq. (3)**
 23 and **Eq. (4)**.

24

$$25 \quad Q_i + \dot{m}_{i+1}^{brine} \cdot H_{i+1}^{brine} = \dot{m}_i^{brine} \cdot H_i^{brine} + \dot{m}_i^{vapor} \cdot H_i^{vapor} \quad \forall i < I \quad (3)$$

$$26 \quad Q_i + \dot{m}_{in}^{feed} \cdot H_i^{feed} = \dot{m}_i^{brine} \cdot H_i^{brine} + \dot{m}_i^{vapor} \cdot H_i^{vapor} \quad \forall i = I \quad (4)$$

1 In which, Q_i indicates the heat flow supplied to system boundary by the
 2 condensed vapor. The specific enthalpies of brine, feed water and boiling vapor
 3 are estimated via correlations as presented in the **Appendix**. Note that brine and
 4 vapor are both at the same boiling temperature $T_i^{boiling}$ in the effect $i \in I$. The
 5 latter is evaluated by considering the boiling point elevation (BPE) over the ideal
 6 temperature in the evaporation effect i as follows.

$$7 \quad T_i^{boiling} = T_i^{ideal} + BPE_i \quad \forall i \in I \quad (5)$$

9
 10 In which, BPE_i and ideal temperature T_i^{ideal} in the effect $i \in I$ are estimated
 11 by the correlations provided in the **Appendix**.

12 The energy requirements in evaporator effects $i \in I$ are given by the
 13 following equations.

$$14 \quad Q_i = \dot{m}^{sup} \cdot Cp_i^{vapor} \cdot (T^{sup} - T_i^{condensate}) + \dot{m}^{sup} \cdot (H_i^{cv} - H_i^{condensate}) + Q^{external} \quad \forall i = 1 \quad (6)$$

$$15 \quad Q_i = \lambda_i \cdot (\dot{m}_{i-1}^{vapor} + \dot{m}_{c_{i-1}}^{vapor}) \quad \forall i > 1 \quad (7)$$

16
 17
 18 In the evaporator effect $i = 1$, energy requirements embrace the sensible
 19 heat needed to achieve the outlet temperature of the condensate, and the latent
 20 heat of condensation of the superheated vapor. In other evaporator effects, the
 21 energy requirements are calculated by the latent heat of vaporization added to
 22 the effect by the boiling vapor and flashed off condensate vapor. In **Eq. (6)**,
 23 $Q^{external}$ represents the energy from a steam external source that is used to avoid
 24 equipment oversizing. This energy amount is estimated as follows.

$$25 \quad Q^{external} = \dot{m}^{steam} \cdot Cp^{vapor} \cdot (T^{steam} - T_i^{condensate}) + \dot{m}^{steam} \cdot (H_i^{cv} - H_i^{condensate}) \quad \forall i = 1$$

26
 27 (8)

In **Eq. (6)** and **Eq. (8)**, the specific enthalpies for vapor H_i^{cv} and condensate $H_i^{condensate}$ phases are given by the correlations presented in the **Appendix**. Note that the condensate temperature $T_i^{condensate}$ in effects $i \in I$ is obtained by considering the outlet vapor pressure of the mechanical compressor in the Antoine Equation (please see the **Appendix**).

In **Eq. (6)**, \dot{m}^{sup} is the superheated mass flowrate as given by the following equation.

$$\dot{m}^{sup} = \dot{m}_{c_i}^{vapor} + \dot{m}_{c_i}^{vapor} \quad \forall i = I \quad (9)$$

In which, $\dot{m}_{c_i}^{vapor}$ and $\dot{m}_{c_i}^{vapor}$ are mass flowrates of the flashed off and boiling vapor from the condensate in evaporator effects $i \in I$, correspondingly.

The total heat transfer area of the evaporator unit of is obtained by the sum of the corresponding areas of each effect as shown in the **Eq. (10)**.

$$A^{evaporator} = \sum_{i=1}^I A_i \quad \forall i \in I \quad (10)$$

In evaporator effect $i = 1$, the heat transfer area should correspond to the sum of the areas related to the latent and sensible heat transfer:

$$A_i = \left[\begin{array}{l} \dot{m}^{sup} \cdot C p_i^{vapor} \cdot (T^{sup} - T_i^{condensate}) / (U^S \cdot LMTD_i) + \\ \dot{m}^{sup} \cdot (H_i^{cv} - H_i^{condensate}) / U_i \cdot (T_i^{condensate} - T_i^{boiling}) \end{array} \right] \quad \forall i = 1 \quad (11)$$

For remaining evaporator effects, the following equation is used to estimate the heat transfer area:

$$A_i = Q_i / (U_i \cdot LMTD_i) \quad \forall i > 1 \quad (12)$$

In which, U_i is the overall heat transfer coefficient that is given by the following correlation (Al-Mutaz and Wazeer, 2014).

$$U_i = 0.001 \cdot \left[\frac{1939.4 + 1.40562 \cdot T_i^{boiling} - 0.00207525 \cdot (T_i^{boiling})^2}{0.0023186 \cdot (T_i^{boiling})^3} + \right] \quad \forall i \in I \quad (13)$$

In **Eq. (11)** and **Eq. (12)**, $LMTD_i$ indicates the log mean temperature difference in evaporator effect $i \in I$. The latter is estimated by using the Chen's approximation (Chen, 1987) for avoiding numerical difficulties related to the temperature differences.

$$LMTD_i = \left[0.5 \cdot (\theta_{1i} \cdot \theta_{2i}) \cdot (\theta_{1i} + \theta_{2i}) \right]^{\frac{1}{3}} \quad \forall i \in I \quad (14)$$

In which,

$$\theta_{1i} = \begin{cases} T_i^{sup} - T_i^{boiling} & \forall i = 1 \\ T_i^{sat} - T_i^{boiling} & \forall i > 1 \end{cases} \quad \theta_{2i} = \begin{cases} T_i^{condensate} - T_{i+1}^{boiling} & \forall i = 1 \\ T_i^{sat} - T_{i+1}^{boiling} & \forall 1 < i < I \\ T_i^{sat} - T_i^{feed} & \forall i = I \end{cases} \quad (15)$$

The following constraint is used to ensure the pressure feasibility in evaporation effects $i \in I$.

$$P_i^{vapor} \geq P_{i+1}^{vapor} + \Delta P_{min} \quad \forall i < I \quad (16)$$

In which the vapor pressure P_i^{vapor} should equal the pressure of saturated vapor from subsequent effect to avoid operating instabilities:

$$P_i^{vapor} = P_{i+1}^{sat} \quad \forall i < I \quad (17)$$

1 Finally, the following temperature constraints are considered to avoid
 2 temperature crossovers in evaporator effects $i \in I$.

$$\begin{cases}
 T_i^{sup} \geq T_i^{condensate} + \Delta T_{min}^1 & \forall i = 1 \\
 T_{i-1}^{boiling} \geq T_i^{condensate} + \Delta T_{min}^1 & \forall i > 1 \\
 T_i^{boiling} \geq T_{i+1}^{boiling} + \Delta T_{min}^2 & \forall i < I \\
 T_i^{boiling} \geq T_i^{feed} + \Delta T_{min}^2 & \forall i = I \\
 T_i^{condensate} \geq T_{i+1}^{boiling} + \Delta T_{min}^3 & \forall i < I \\
 T_i^{condensate} \geq T_i^{feed} + \Delta T_{min}^3 & \forall i = I \\
 T_i^{condensate} \geq T_i^{boiling} + \Delta T_{min}^4 & \forall i \in I \\
 T_i^{sat} \geq T_i^{boiling} + \Delta T_{min}^4 & \forall i \in I
 \end{cases} \quad (18)$$

4

5 4.1.2. Flashing Tanks

6 The mass balances in the flashing unit of the evaporator effect i can be expressed
 7 as follows.

8

$$9 \quad \dot{m}^{sup} = \dot{m}_{c_i}^{vapor} + \dot{m}_{c_i}^{liquid} \quad \forall i = 1 \quad (19)$$

$$10 \quad \dot{m}_{i-1}^{vapor} + \dot{m}_{c_{i-1}}^{vapor} + \dot{m}_{c_{i-1}}^{liquid} = \dot{m}_{c_i}^{vapor} + \dot{m}_{c_i}^{liquid} \quad \forall i > 1 \quad (20)$$

11

12 In which, $\dot{m}_{c_i}^{vapor}$ and $\dot{m}_{c_i}^{liquid}$ represent the mass flowrates of vapor and liquid
 13 phases of the flashed off condensate in the effect $i \in I$, respectively.

14 The energy balances in the flashing unit of the evaporator effect i are
 15 given by the following equations.

16

$$17 \quad \dot{m}^{sup} \cdot H_i^{condensate} = \dot{m}_{c_i}^{vapor} \cdot H_{c_i}^{vapor} + \dot{m}_{c_i}^{liquid} \cdot H_{c_i}^{liquid} \quad \forall i = 1 \quad (21)$$

$$18 \quad (\dot{m}_{i-1}^{vapor} + \dot{m}_{c_{i-1}}^{vapor}) \cdot H_i^{condensate} + \dot{m}_{c_{i-1}}^{liquid} \cdot H_{c_{i-1}}^{liquid} = \dot{m}_{c_i}^{vapor} \cdot H_{c_i}^{vapor} + \dot{m}_{c_i}^{liquid} \cdot H_{c_i}^{liquid} \quad \forall i > 1 \quad (22)$$

19

20 In which, $H_{c_i}^{vapor}$ and $H_{c_i}^{liquid}$ are the specific enthalpies for vapor and liquid
 21 phases of the flashed off condensate in the effect $i \in I$, respectively. They are
 22 estimated at the ideal temperature via correlations as presented in the **Appendix**.

1 The volume of the flashing unit of the evaporator effect i is determined by
 2 **Eq. (23)** and **Eq. (24)**.

$$3 \quad V_i^{flash} = (\dot{m}^{sup} \cdot rt) / \rho_i \quad \forall i = 1 \quad (23)$$

$$4 \quad V_i^{flash} = (\dot{m}_{i-1}^{vapor} + \dot{m}_{c_{i-1}}^{liquid}) \cdot rt / \rho_i \quad \forall i > 1 \quad (24)$$

5
 6 In which, rt and ρ_i indicate the time of retention in the flashing tank and
 7 condensate density, correspondingly. In this study, we consider a retention time
 8 of 5 min.

9 10 4.1.3. Mechanical Vapor Compressor

11 The outlet isentropic temperature of the mechanical vapor compressor is given
 12 as follows.

$$14 \quad T^{is} = (T_i^{mix} + 273.15) \cdot (P^{sup} / P_i^{vapor})^{\frac{\gamma-1}{\gamma}} - 273.15 \quad \forall i = I \quad (25)$$

15
 16 In **Eq. (25)**, T_i^{mix} indicates the temperature of mixture obtained from an
 17 energy balance of the mixer in the last evaporator effect $i = I$. P^{sup} is the pressure
 18 of superheated vapor, which is limited by the maximum compression ratio CR_{max}
 19 as expressed by **Eq. (26)**.

$$21 \quad P^{sup} \leq CR_{max} \cdot P_i^{vapor} \quad \forall i = I \quad (26)$$

22
 23 The temperature of the superheated vapor from the mechanical vapor
 24 compressor is estimated by **Eq. (27)**.

$$26 \quad T^{sup} = T_i^{mix} + \frac{1}{\eta_{IS}} \cdot (T^{IS} - T_i^{mix}) \quad \forall i = I \quad (27)$$

1

2 In which, η^{IS} represents the isentropic efficiency of the compressor.

3 The compressor mechanical power is given by the following equation.

4

5
$$W^{compressor} = \dot{m}^{sup} \cdot (H^{sup} - H_i^{vapor}) \quad \forall i = I \quad (28)$$

6

7 In which, H^{sup} and H_i^{vapor} are specific enthalpies of vapor evaluated at
8 superheated and mixture temperatures, respectively. The correlations of vapor
9 specific enthalpies are shown in the **Appendix**. The following constraints on the
10 superheated temperature and pressure are used to guarantee the proper
11 operation of the compressor.

12

13
$$T^{sup} \geq T_i^{mix} \quad \forall i = I \quad (29)$$

14
$$P^{sup} \geq P_i^{vapor} \quad \forall i = I \quad (30)$$

15

16

4.1.4. Feeding Preheater

17 The global energy balance in the feeding preheater unit is stated as follows.

18

19
$$\dot{m}_{c_i}^{liquid} \cdot Cp_i^{condensate} \cdot (T_i^{ideal} - T_{out}^{freshwater}) = \dot{m}_{in}^{feed} \cdot Cp_{in}^{feed} \cdot (T_i^{feed} - T_{in}^{feed}) \quad \forall i = I \quad (31)$$

20

21 In which, T_{in}^{feed} and $T_{out}^{freshwater}$ are temperatures of the feed water and
22 produced freshwater by the system, correspondingly. The specific heats of the
23 condensate and feed water are obtained via correlations as presented in the
24 **Appendix**.25 The heat transfer area of the feeding preheater is given by **Eq. (32)**.

26

27
$$A^{preheater} = \dot{m}_{c_i}^{liquid} \cdot Cp_i^{condensate} \cdot (T_i^{ideal} - T_{out}^{freshwater}) / (U \cdot LMTD) \quad \forall i = I \quad (32)$$

1
2 In which, U represents the overall heat transfer coefficient at T_i^{ideal} as
3 estimated by **Eq. (13)**. The logarithmic mean temperature difference $LMTD$ is
4 obtained by **Eq. (14)**. In this case, the temperature differences are stated as
5 follows.

$$6 \quad \begin{cases} \theta_1 = T_i^{ideal} - T_i^{feed} & \forall i = I \\ \theta_2 = T_{out}^{freshwater} - T_{in}^{feed} \end{cases} \quad (33)$$

8 9 *4.1.5. Zero-Liquid Discharge Specification*

10 The zero-liquid discharge operation of the thermal desalination system is ensured
11 by the following design constraint.

$$12 \quad S_i^{brine} \geq S^{design} \quad \forall i = 1 \quad (34)$$

15 **4.2. Modelling of the Steam Rankine Cycle**

16 The thermal efficiency of the steam Rankine cycle is given by the following
17 equation.

$$18 \quad \eta^{RC} = \frac{W^{RC}}{Q^{Boiler}} \quad (35)$$

20
21 In which, W^{RC} represents the net power of the Rankine cycle, while Q^{Boiler}
22 is the thermal power of the boiler. The following inequality constraint is required
23 to couple the steam Rankine cycle to the MEE-MVR desalination system.

$$24 \quad W^{RC} \geq W^{compressor} \quad (36)$$

26

1 In which, **Eq. (36)** is used to ensure that net power provided by the Rankine
2 cycle is higher or equal to the power needed to drive the compressor in the
3 desalination system. The net power of the Rankine cycle is given as follows.

$$4 \quad W^{RC} = W^{turbine} - W^{RC_pump} \quad (37)$$

6
7 In which, $W^{turbine}$ and W^{RC_pump} represent the mechanical power produced
8 by the steam turbine and consumed by the pump in the Rankine cycle,
9 respectively. The modelling equations of the steam turbine, pump, and condenser
10 of the steam Rankine cycle are presented in the next sections.

11 12 4.2.1. Steam Turbine

13 The mechanical power produced by the steam turbine is given by the following
14 equation.

$$15 \quad W^{turbine} = \dot{m}^{RC} \cdot (H_{in}^{turbine} - H_{out}^{turbine}) \quad (38)$$

17
18 In **Eq. (38)**, \dot{m}^{RC} indicates the mass flowrate of the working fluid (water) in
19 the Rankine cycle, which is constant throughout the cycle. $H_{in}^{turbine}$ and $H_{out}^{turbine}$ are
20 the specific enthalpies of the working fluid at the inlet and outlet of the turbine,
21 respectively. The specific enthalpy of vapor at the turbine outlet $H_{out}^{turbine}$ is
22 estimated from the definition of isentropic efficiency η^{IS} as follows.

$$23 \quad H_{out}^{turbine} = H_{in}^{turbine} - \eta^{IS} \cdot (H_{in}^{turbine} - H_{out}^{IS}) \quad (39)$$

24
25
26 The isentropic enthalpy of the humid vapor at the turbine outlet is defined
27 as follows.

28

$$1 \quad H_{out}^{IS} = H_{out}^L - x^{IS} \cdot (H_{out}^V - H_{out}^L) \quad (40)$$

2

3 The vapor quality in the isentropic expansion process, and the actual vapor
4 quality at the turbine outlet are given the following expressions.

$$5 \quad x^{IS} = \frac{S_{out}^{turbine} - S_{out}^L}{S_{out}^V - S_{out}^L} \quad (41)$$

$$6 \quad x_{out}^{turbine} = \frac{H_{out}^{turbine} - H_{out}^L}{H_{out}^V - H_{out}^L} \quad (42)$$

7

8 The specific enthalpies and entropies of liquid and vapor states at the
9 turbine outlet are estimated by the following correlations (Lemmon et al., 1980;
10 National Institute of Standards, 2011).

11

$$12 \quad H_{out}^L = a_{hL} + b_{hL} \cdot T^{sat} + c_{hL} \cdot (T^{sat})^2 + d_{hL} \cdot (T^{sat})^3 + e_{hL} \cdot (T^{sat})^4 + f_{hL} \cdot (T^{sat})^5 \quad (43)$$

$$13 \quad H_{out}^V = a_{hV} + b_{hV} \cdot T^{sat} + c_{hV} \cdot (T^{sat})^2 + d_{hV} \cdot (T^{sat})^3 + e_{hV} \cdot (T^{sat})^4 + f_{hV} \cdot (T^{sat})^5 \quad (44)$$

14

$$15 \quad s_{out}^L = a_{sL} + b_{sL} \cdot T^{sat} + c_{sL} \cdot (T^{sat})^2 + d_{sL} \cdot (T^{sat})^3 + e_{sL} \cdot (T^{sat})^4 + f_{sL} \cdot (T^{sat})^5 \quad (45)$$

$$16 \quad s_{out}^V = a_{sV} + b_{sV} \cdot T^{sat} + c_{sV} \cdot (T^{sat})^2 + d_{sV} \cdot (T^{sat})^3 + e_{sV} \cdot (T^{sat})^4 + f_{sV} \cdot (T^{sat})^5 \quad (46)$$

17

18 The following inequality constraints are used to guarantee the temperature
19 and pressure feasibility in the steam turbine.

20

$$21 \quad \begin{cases} T_{out}^{turbine} \leq T_{in}^{turbine} \\ T_{in}^{turbine} \geq T_{in}^{sat} \\ P_{out}^{sat} \leq P_{in}^{sat} \end{cases} \quad (47)$$

22

1 The pressure of vapor in saturation conditions is obtained from the
2 modified version of the Antoine equation as available in the process simulator
3 Aspen HYSYS.

$$4 \quad P^{sat} = \exp\left(A + \frac{B}{C + T^{sat}} + D \cdot \ln(T^{sat}) + E \cdot (T^{sat})^F\right) \quad (48)$$

6 4.2.2. Rankine Cycle Pump

7 The power consumed by the pump in the Rankine cycle is estimated as follows.

$$8 \quad W^{RC_pump} = \frac{\dot{m}^{RC} \cdot v \cdot (P_{in}^{sat} - P_{out}^{sat})}{\eta^{RC_pump}} \quad (49)$$

10
11 In which, v represents the specific volume of liquid water, while η^{RC_pump}
12 indicates the RC pump efficiency. The specific enthalpy of the working fluid at the
13 pump outlet is obtained by the following equation.

$$14 \quad H_{out}^{RC_pump} = H_{in}^{RC_pump} + v \cdot (P_{in}^{sat} - P_{out}^{sat}) \quad (50)$$

16
17 Note that the properties at the inlet of the pump should correspond to
18 those at the condenser outlet in the Rankine cycle. Hence, $H_{in}^{RC_pump} = H_{out}^{condenser}$.

19 4.2.3. Condenser

20 The thermal power of the condenser in the Rankine cycle is given as follows.

$$21 \quad Q^{condenser} = \dot{m}^{RC} \cdot (H_{in}^{condenser} - H_{out}^{condenser}) \quad (51)$$

22
23
24
25 In which, $H_{in}^{condenser}$ and $H_{out}^{condenser}$ are the specific enthalpies of the working
26 fluid at the inlet and outlet of the condenser, respectively. Note that the

1 properties at the inlet of the condenser should correspond to those at the turbine
2 outlet. Hence, $H_{in}^{condenser} = H_{out}^{turbine}$.

3 The heat transfer area of the condensed can be obtained by the following
4 equation.

$$6 \quad A^{condenser} = \frac{Q^{condenser}}{U^{condenser} \cdot LMTD^{condenser}} \quad (52)$$

7 In which, $U^{condenser}$ indicates the heat transfer coefficient. The logarithmic
8 mean temperature difference $LMTD^{condenser}$ is obtained through the Chen's
9 approximation as given by **Eq. (14)** (Chen, 1987). In this case, the temperature
10 differences are stated as follows.

$$12 \quad \begin{cases} \theta_1 = T_{in}^{condenser} - T_{out} \\ \theta_2 = T_{out}^{condenser} - T_{in} \end{cases} \quad (53)$$

13 In which,

$$14 \quad \begin{cases} T_{in}^{condenser} \geq T_{out} + \Delta T_{min} \\ T_{out}^{condenser} \geq T_{in} + \Delta T_{min} \end{cases} \quad (54)$$

15
16 The thermal power required by the Rankine cycle to generate super-heated
17 steam in the boiler outlet is provided by heat exchanges with the solar thermal
18 system. The modelling equations for the solar thermal system are presented as
19 follows.

21 **4.3. Modelling of the Solar Thermal System**

22 The solar thermal system is designed to operate in different time periods, which
23 account for the daily solar radiation flux (irradiance) throughout the year. Thus,
24 the following index set is needed to develop the multi-period model for the solar
25 thermal system design.

$$T = \{t / t = 1, 2, \dots, T \text{ is a time period}\}$$

The heat demands of the boiler are provided by the solar collectors' field and a backup gas-fired heater. Therefore, the global energy balance in the solar thermal system is expressed as follows.

$$Q_t^{boiler} = Q_t^{SC} + Q_t^{GFH} \quad \forall t \in T \quad (55)$$

In which, Q_t^{boiler} , Q_t^{SC} and Q_t^{GFH} refer to the thermal power of the boiler, solar collectors field, and gas-fired heater in the time period $t \in T$, respectively.

The mass balances at each node of the solar thermal system are given by the following formulation.

$$\begin{cases} \dot{m}_{out,t}^{boiler} = \dot{m}_{in,t}^{SC} + \dot{m}_{in,t}^{GFH} \\ \dot{m}_{in,t}^{boiler} = \dot{m}_{out,t}^{SC} + \dot{m}_{out,t}^{GFH} \\ \dot{m}_{in,t}^{boiler} = \dot{m}_{out,t}^{boiler} \\ \dot{m}_{in,t}^{SC} = \dot{m}_{out,t}^{SC} \\ \dot{m}_{in,t}^{GFH} = \dot{m}_{out,t}^{GFH} \end{cases} \quad \forall t \in T \quad (56)$$

The energy balances at each node of the solar thermal system are given by the following formulation.

$$\begin{cases} \dot{m}_{out,t}^{boiler} \cdot H_{out,t}^{boiler} = \dot{m}_{in,t}^{SC} \cdot H_{in,t}^{SC} + \dot{m}_{in,t}^{GFH} \cdot H_{in,t}^{GFH} \\ \dot{m}_{in,t}^{boiler} \cdot H_{in,t}^{boiler} = \dot{m}_{out,t}^{SC} \cdot H_{out,t}^{SC} + \dot{m}_{out,t}^{GFH} \cdot H_{out,t}^{GFH} \\ H_{out,t}^{boiler} = H_{in,t}^{SC} \\ H_{out,t}^{boiler} = H_{in,t}^{GFH} \end{cases} \quad \forall t \in T \quad (57)$$

In which the specific enthalpies of the heating fluid (oil Therminol 72) at the inlet and outlet of each solar thermal system equipment are estimated as follows.

$$1 \quad H_t = Cp^{hf} \cdot T_t \quad \forall t \in T \quad (58)$$

2

3 In which, Cp^{hf} indicates the specific heat, and T_t the temperature of the
4 heating fluid in the time period $t \in T$.

5

6 4.3.1. Solar Thermal Collectors

7 The thermal power produced by the solar collectors' field in the time period $t \in T$
8 is given by **Eq. (59)**.

9

$$10 \quad Q_t^{SC} = \dot{m}_{in,t}^{SC} \cdot (H_{out,t}^{SC} - H_{in,t}^{SC}) \quad \forall t \in T \quad (59)$$

11

12 The total area of the solar parabolic trough collectors is estimated as
13 follows.

14

$$15 \quad A^{SC} \geq \frac{Q_t^{SC}}{G_t \cdot \eta^{SC}} \quad \forall t \in T \quad (60)$$

16

17 In **Eq. (60)**, G_t is the daily solar radiation flux (irradiance) in the time period
18 $t \in T$. Also, η^{SC} is the thermal efficiency of the medium-high temperature solar
19 parabolic trough collectors as given by the following expression (Salcedo et al.,
20 2012).

21

$$22 \quad \eta^{SC} = \eta_0 - a_1 \cdot (T_t^{avg} - T_t^{amb}) - a_2 \cdot \left(\frac{T_t^{avg} - T_t^{amb}}{G_t} \right) - a_3 \cdot \left(\frac{T_t^{avg} - T_t^{amb}}{G_t} \right)^2 \quad \forall t \in T \quad (61)$$

23

24 In which, η_0 is the collector optical efficiency, while a_1 , a_2 , and a_3 are
25 coefficients. T_t^{amb} and T_t^{avg} are the ambient and average temperatures in the time
26 period $t \in T$, respectively. The average temperature of the solar collectors is
27 calculated as follows.

$$T_t^{avg} = 0.5 \cdot (T_{in,t}^{SC} + T_{out,t}^{SC}) \quad \forall t \in T \quad (62)$$

2

3 4.3.2. Gas-Fired Heater

4 The thermal power produced by the natural gas-fired heater in the time period
5 $t \in T$ is estimated as follows.

$$Q_t^{GFH} = \dot{m}_t^{ng} \cdot LHV \cdot \eta^{GFH} \quad \forall t \in T \quad (63)$$

7

8 In which, \dot{m}_t^{ng} and LHV indicate the mass flowrate and lower heating value
9 of natural gas, respectively. η^{GFH} is the thermal efficiency of the natural gas heater.

10

11 4.3.3. Boiler

12 The thermal power of the boiler in the time period $t \in T$ is given as follows.

13

$$Q_t^{boiler} = \dot{m}_{in,t}^{boiler} \cdot (H_{in,t}^{boiler} - H_{out,t}^{boiler}) \quad \forall t \in T \quad (64)$$

15

16 The heat transfer area of the boiler can be estimated by the following equation.

17

$$A^{boiler} = \frac{Q_t^{boiler}}{U^{boiler} \cdot LMTD_t^{boiler}} \quad (65)$$

19

20 In which, U^{boiler} indicates the heat transfer coefficient. The logarithmic
21 mean temperature difference $LMTD_t^{boiler}$ in the time period $t \in T$ is obtained
22 through the Chen's approximation as given by **Eq. (14)** (Chen, 1987). In this case,
23 the temperature differences are stated as follows.

24

$$\begin{cases} \theta_1 = T_{in,t}^{boiler} - T_{in}^{turbine} \\ \theta_2 = T_{out,t}^{boiler} - T_{out}^{RC_pump} \end{cases} \quad (66)$$

26 In which,

$$\begin{cases} T_{in,t}^{boiler} \geq T_{in}^{turbine} + \Delta T_{min} \\ T_{out,t}^{boiler} \geq T_{out}^{RC_pump} + \Delta T_{min} \end{cases} \quad (67)$$

2

3 **4.4. Economic and Environmental Objective Functions**

4 As mentioned before, the multi-objective NLP-based model is optimized via the
5 simultaneous minimization of economic and environmental objective functions.

6 These objective functions are presented in the following sections.

7

8 *4.4.1. Economic Performance Evaluation*

9 The economic objective function corresponds to the minimization of the total
10 annualized cost of the solar-assisted MEE-MVR system. The total annualized cost
11 (*TAC*) is composed of the total capital investment (*CAPEX*) in all system devices,
12 and total operating and maintenance expenses (*OPEX*) as stated as follows.

13

$$14 \quad TAC = CAPEX + OPEX \quad (68)$$

15

16 The total capital investment comprises the costs of all equipment units
17 from the MEE-MVR desalination system, steam Rankine cycle, and solar thermal
18 system:

19

$$20 \quad CAPEX = CAPEX^{MEE-MVR} + CAPEX^{RC} + CAPEX^{STS} \quad (69)$$

21

22 In which,

$$23 \quad CAPEX^{MEE-MVR} = fac \cdot \left(\frac{CEPCI^{2019}}{CEPCI^{2003}} \right) \cdot \left[\begin{aligned} & (C_{PO} \cdot F_{BM} \cdot F_P)^{evaporator} + (C_{PO} \cdot F_{BM} \cdot F_P)^{compressor} + \\ & \left(\sum_{i=1}^I C_{POi} \cdot F_{BM} \cdot F_P \right)^{flashing} + (C_{PO} \cdot F_{BM} \cdot F_P)^{preheater} \end{aligned} \right]$$

24 (69a)

$$25 \quad CAPEX^{RC} = fac \cdot \left(\frac{CEPCI^{2019}}{CEPCI^{2003}} \right) \cdot \left[\begin{aligned} & (C_{PO} \cdot F_{BM} \cdot F_P)^{turbine} + (C_{PO} \cdot F_{BM} \cdot F_P)^{condenser} + \\ & (C_{PO} \cdot F_{BM} \cdot F_P)^{RC_Pump} \end{aligned} \right] \quad (69b)$$

$$1 \quad CAPEX^{STS} = f_{ac} \cdot \left(\frac{CEPCI^{2019}}{CEPCI^{2003}} \right) \cdot \left[(C_{PO} \cdot F_{BM} \cdot F_P)^{boiler} + (C_{PO} \cdot F_{BM} \cdot F_P)^{SC} + \right. \\ \left. (C_{PO} \cdot F_{BM} \cdot F_P)^{GFH} + (C_{PO} \cdot F_{BM} \cdot F_P)^{STS_Pump} \right] \quad (69c)$$

2

3 In the previous formulation, f_{ac} represents the annualization factor for the
4 capital investment cost as defined by Smith (2005):

5

$$6 \quad f_{ac} = \frac{fi \cdot (1 + fi)^y}{(1 + fi)^y - 1} \quad (70)$$

7

8 In which, fi indicates the fractional interest rate per year, and y refers to
9 the number of years in the amortization period. In **Eq. (69a) – Eq. (69c)**, C_{PO}
10 represents the basic cost of a unitary equipment (in kUS\$) that operates at near-
11 ambient pressure conditions. This unitary cost is obtained from cost correlations
12 as proposed by Turton et al. (2012) and Couper et al. (2010). In addition, F_{BM} is
13 the correction factor of the basic unitary cost, which accounts for the operating
14 pressure and construction materials. Note that the total annualized cost is
15 corrected for the relevant year through the CEPCI index (Chemical Engineering
16 Plant Cost Index).

17 The operating and maintenance expenses embraces the cost of utilities
18 (e.g., natural gas, cooling water, and electricity), and equipment maintenance as
19 stated as follows.

20

$$21 \quad OPEX = \left[\underbrace{C^{CW} \cdot Q^{condenser} + C^{electricity} \cdot \sum_{t \in T} W_t^{STS_pump} + C^{NG} \cdot \sum_{t \in T} Q_t^{GFH}}_{\text{operating expenses}} + \right. \\ \left. \underbrace{0.25 \cdot CAPEX^{RC} + 0.15 \cdot CAPEX^{STS}}_{\text{equipment maintenance}} \right] \quad (71)$$

22

23 In which, C^{CW} , $C^{electricity}$, and C^{NG} are cost parameters for cooling water,
24 electricity, and natural gas, respectively. In this study, the maintenance expenses

1 of the Rankine cycle units are considered to be equal to 25% of the corresponding
2 capital costs, while the maintenance expenses of the STS correspond to 15% of
3 the capital costs of the same units.

4 5 4.4.2. Environmental Performance Evaluation

6 The environmental objective function accounts for the environmental impacts
7 associated with utilities consumption, which include electricity (STS pump),
8 natural gas (GFH), and cooling water (condenser). In this study, the environmental
9 impacts are quantified by the LCA-based ReCiPe methodology (Goedkoop et al.,
10 2009). The quantification of environmental impacts is performed by LCA through
11 four key stages. Firstly, the goal and scope are defined. The ReCiPe methodology
12 accounts for 17 different categories of midpoint level impacts that are divided
13 into three main damage groups at end level. Then, the Life Cycle Inventory (LCI)
14 is carried out to appraise all material inputs and outputs, as well as energy inputs
15 and outputs. In the third stage, the Life Cycle Impact Assessment (LCIA) is used to
16 evaluate, weight and quantify the environmental impacts into eco-points. The
17 environmental objective function is expressed by the following equation.

$$19 \quad EI = LCIA^{electricity} \cdot \sum_{t \in T} W_t^{STS_pump} + LCIA^{NG} \cdot \sum_{t \in T} Q_t^{GFH} + LCIA^{CW} \cdot Q^{condenser} \quad (72)$$

20
21 In which, $LCIA^{electricity}$, $LCIA^{NG}$, and $LCIA^{CW}$ denote the environmental impacts
22 points (eco-points) related to the electricity used by the STS pump, natural gas
23 consumed by the GFH, and cooling water required by the condenser, respectively.
24 The environmental impacts are estimated through total ReCiPe points per year as
25 obtained from the Ecoinvent database (Ecoinvent default, LCIA, ReCiPe Endpoint
26 H/A, Europe/Es). A plant operating time of 8760 h/year is considered to convert
27 original eco-points per energy production units into points per kW year units. The
28 impacts associated with the stage of system construction are neglected as they

1 are usually much smaller than those related to the operation during the system
2 lifetime.

3

4 **4.5. Optimization Procedure: Epsilon-Constraint Method**

5 The multi-objective NLP problem can be formally expressed as follows.

6

$$\begin{aligned} 7 \quad & \min \quad \{TAC, EI\} \\ & s.t. \quad \text{all equality and inequality constraints} \end{aligned} \quad (73)$$

8

9 In which, *TAC* denotes the total annualized cost as given by **Eq. (68)**, while
10 *EI* represents the total environmental impact as estimated by **Eq. (72)**. The multi-
11 objective mathematical model was implemented in GAMS software (Rosenthal,
12 2016) (version 26.1.0), and solved via the epsilon-constraint method (Ehrgott,
13 2005). The epsilon-constraint method consists of formulating an auxiliary single-
14 objective model, in which one objective is expressed as the main goal whilst the
15 other objective is stated as an additional constraint. Then, the single-objective
16 model is solved several times for different epsilon bound values that are imposed
17 on the problem constraints. This approach allows obtaining a different optimal
18 solution for each of the considered epsilon bound values. Hence, a Pareto curve
19 can be constructed to show the set of alternative solutions, where each solution
20 represents an optimal trade-off between the economic and environmental
21 objective functions (García et al., 2012; Mavrotas, 2009). The local optimizer
22 CONOPT4 was applied to optimize the multi-objective NLP problem with CPU
23 time of ~2 min (180 different time periods and 30 Pareto-optimal solutions).

24

25 **5. Case Study**

26 An illustrative case study is carried out to assess the effectiveness of the
27 developed approach for the multi-objective optimization of solar-based ZLD

1 desalination systems. The decentralized system is composed of an STS, Rankine
2 cycle unit, and a MEE-MVR desalination plant. **Fig. 1** depicts the schematic
3 diagram for the solar-driven MEE-MVR system as proposed for the ZLD
4 desalination of high-salinity shale gas wastewaters. The treatment capacity of the
5 MEE-MVR desalination plant is equal to 10.42 kg/s of shale gas wastewater. The
6 salt concentration (salinity) of the feed water is considered to be equal to 70 g/kg,
7 and its inlet temperature is 25°C. For ensuring the ZLD operation, the brine salinity
8 should achieve a minimum value of 300 g/kg (300k ppm) at the system discharge
9 (Han et al., 2017). **Table 1** shows the process and cost parameters used in the
10 mathematical modelling formulation of the zero-liquid discharge MEE-MVR
11 system. Additional data encompass operational limitations on the saturation
12 pressure (200 kPa) and ideal temperature (100°C) to avoid rusting and fouling-
13 related problems in the evaporator. The latter is a horizontal-tube falling film unit,
14 which is built of nickel. A minimum temperature approach of 2°C is considered to
15 prevent temperature crossovers in the evaporator effects. Besides, minimum
16 temperature and pressure drops equal to 0.1°C and 0.1 kPa, respectively, are used
17 between two successive evaporation effects. The maximum compression ratio is
18 limited to 3 in the mechanical vapor compressor (centrifugal/carbon steel), whilst
19 the heat capacity ratio is 1.33 (Onishi et al., 2017a, 2017b, 2017c).

20 In the STS, solar parabolic trough collectors are considered owing to their
21 greater efficiencies at high temperatures. The thermal fluid is Therminol 72 due
22 to its high thermal stability at temperatures up to 380°C (Salcedo et al., 2012). The
23 process and cost parameters used for the optimal design of the steam Rankine
24 cycle and STS are presented in **Table 2**. The daily solar irradiance throughout the
25 year in Spain (N 41°7'8", E 1°14'43") is displayed in **Table 3**. The minimum
26 temperature difference in the hot end of the condenser is in a range of 5–15°C,
27 while the temperature increase of the thermal fluid in the boiler is 50°C. Cost
28 parameters include prices of electricity (812.47 US\$ per kW year), and natural gas
29 (277.03 US\$ per kW year), which are retrieved from Eurostat database (2020). The

1 factor of annualized capital cost is equal to 0.163, which corresponds to 10% of
2 interest rate over 10 years of amortization period. **Table 4** presents the
3 environmental impact points of the utilities. The environmental impacts are
4 estimated through total ReCiPe points per year as obtained from the Ecoinvent
5 database. A plant operating time of 8760 h/year is considered to convert original
6 ReCiPe eco-points per energy production units into points per kW year units.

7 Firstly, the problem is solved by considering each optimization single-
8 objective alone. Thus, the optimization is performed via the minimization of the
9 total annualized cost (*TAC*), and the total environmental impacts (*EI*) separately.
10 Note that the minimization of the economic and environmental single-objectives
11 allows obtaining the limits of the epsilon-constraint interval. Then, the latter
12 interval is divided into a set of subintervals and successive optimizations
13 (iterations) are performed through the minimization of the economic objective-
14 function subjected to each environmental upper bound (*i.e.*, epsilon-constraint
15 that ensures that a given environmental limit is not exceeded). By applying the
16 previous epsilon-constraint approach, we obtain a set of optimal trade-off Pareto
17 solutions. The results obtained are discussed as follows.

18

19 **6. Results and Discussion**

20 **6.1. Single-Objective Optimization: EI Minimization**

21 The total annualized cost obtained via the minimization of the environmental
22 objective-function is equal to 45592 kUS\$/year, encompassing 45433 kUS\$/year
23 associated with capital investment, and 159 kUS\$/year related to operating
24 (electricity, natural gas, and cooling water consumption) and maintenance
25 expenses. The capital cost is composed of 2603 kUS\$/year for the investment in
26 the MEE-MVR desalination system, and 42830 kUS\$/year for the STS and RC units.
27 Also, the total environmental impacts related to utilities consumption (electricity,
28 natural gas, and cooling water) are estimated to be ~193k ReCiPe eco-

1 points/year. This single-objective optimal solution corresponds to the extreme
2 solution referred to as "Design A" in **Fig. 2** and **Fig. 3**. In this case, the solar-based
3 desalination system requires a total area of the solar parabolic trough collectors
4 of $5.2 \times 10^5 \text{ m}^2$, and the RC steam turbine produces 502.49 kW of electricity to drive
5 mechanical compressor in the MEE-MVR plant.

6 The optimal MEE-MVR desalination system obtained by the minimization
7 of environmental impacts is composed of two evaporation effects with heat
8 transfers areas of 1268.94 m^2 and 468.64 m^2 . In addition, a feeding preheater with
9 a heat transfer area of 100.28 m^2 (1669.63 kW) is required in the system, along
10 with two flashing tanks with volumes of 1.19 m^3 and 2.39 m^3 . Note that the
11 capacity of the mechanical vapor compressor is equal to 502.49 kW . Under this
12 configuration, the desalination system achieves a freshwater production ratio of
13 7.99 kg/s .

14

15 **6.2. Single-Objective Optimization: TAC Minimization**

16 The total annualized cost obtained via the minimization of the economic
17 objective-function is equal to $2224 \text{ kUS\$/year}$, comprising $1794 \text{ kUS\$/year}$ related
18 to capital investment, and $430 \text{ kUS\$/year}$ associated with operating (electricity,
19 natural gas, and cooling water consumption) and maintenance expenses. The
20 capital cost is composed of $1166 \text{ kUS\$/year}$ for the investment in the MEE-MVR
21 desalination system, and $628 \text{ kUS\$/year}$ for the STS and RC units. Still, the total
22 environmental impacts related to utilities consumption (electricity, natural gas,
23 and cooling water) are estimated to be $\sim 667.5 \text{ k ReCiPe eco-points/year}$. This
24 single-objective optimal solution corresponds to the extreme solution referred to
25 as "Design B" in **Fig. 2** and **Fig. 3**. In this case, the solar-based desalination system
26 requires a total area of the solar parabolic trough collectors of 4942 m^2 , and the
27 RC steam turbine produces 734.68 kW of electricity to drive mechanical
28 compressor in the MEE-MVR plant.

1 The optimal MEE-MVR desalination system obtained by the minimization
2 of the total annualized cost is composed of two evaporation effects with heat
3 transfers areas of 284.54 m² and 297.22 m². In addition, a feeding preheater with
4 a heat transfer area of 68.73 m² (1903.66 kW) is required in the system, along with
5 two flashing tanks with volumes of 1.19 m³ and 2.39 m³. Note that the capacity
6 of the mechanical vapor compressor is equal to 734.68 kW. Under this
7 configuration, the desalination system achieves a freshwater production ratio of
8 7.99 kg/s. The comparison between the two extreme environmental and
9 economic optimal solutions reveals that the total heat transfer area of the
10 evaporator is reduced by ~66.5% when the total annualized cost is minimized.
11 Also, the heat transfer area of the feeding preheater is decreased in ~31.5%.
12 Although the compressor capacity is increased in ~46.2%, the minimization of the
13 TAC leads to a reduction of ~55.2% in the capital cost of the MEE-MVR when
14 compared to the minimum EI solution. The capital cost of investment in the STS
15 and RC units is also decreased in ~98.5%, which is mainly due to the reduction of
16 ~99% in the total area of the solar parabolic trough collectors. It should also be
17 noted that the TAC is reduced in ~95.1% while the EI is increased in 245.9%, when
18 contrasting both extreme optimal solutions.

19

20 **6.3. Multi-Objective Optimization: Pareto Optimal Solutions**

21 The Pareto set of optimal trade-off solutions obtained via the multi-objective
22 optimization procedure are displayed in **Fig. 2**. In this figure, Design A represents
23 the minimum EI solution while Design B indicates the minimum TAC solution. It
24 should be highlighted that each point in the Pareto curve correspond to an
25 optimal system design and associated process operating conditions, which yield
26 a unique combination of environmental and economic performance. Since a
27 given improvement in one criterion can only be attained at the expense of
28 impairing the another one, there is a clear trade-off between environmental and
29 economic objectives. Hence, the minimum EI solution (Design A) shows the worst

1 economic performance whilst the minimum TAC solution leads to the highest
2 environmental impacts. As mentioned before, the TAC of Design A is equal to
3 45592 kUS\$/year, whereas Design B presents a TAC of 2224 kUS\$/year. On the
4 other hand, it is also observed an increase in the environmental impacts from
5 ~193k to 667.5k points/year, when moving from Design A to Design B in the
6 Pareto curve.

7 A thorough examination of **Fig. 2** also reveals that the environmental
8 impacts are significantly reduced by increasing the area of the solar parabolic
9 trough collectors. However, as previously discussed, such EI reduction comes with
10 a considerable increase in the total annualized cost of the system. For further
11 analysis, we solved the model by fixing the solar collector area to zero. In this
12 solution, the TAC of the system is equal to 2243 kUS\$/year, whereas the EI are
13 estimated to be 992.3k points/year. The TAC is slightly higher than that of Design
14 B due to the increase in both the capital cost of investment in the MEE-MVR
15 desalination system, and operating expenses related to the larger consumption
16 of natural gas. Clearly, the latter result is also responsible for an increase of
17 ~48.7% in the environmental impacts of the system. Therefore, using solar
18 thermal collectors to drive the MEE-MVR desalination plant is not only an
19 environment-friendly solution but also an economically viable one.

20 Since Design A and Design B correspond to extreme solutions in the Pareto
21 Curve (which can be prohibitive either in terms of high process costs or excessive
22 environmental impacts), we identify Design C as a promising alternative optimal
23 solution. In this case, the TAC of the system is equal to 6867 kUS\$/year, while the
24 total EI related to utilities consumption (electricity, natural gas, and cooling water)
25 is equal to 209.6k ReCiPe eco-points/year. Thus, it is possible to decrease the TAC
26 in ~85% at expense of only 8.5% of increase in environmental impacts when
27 moving from Design A to Design C. The decrease in the TAC is mainly due to the
28 reduction of total area of the solar parabolic trough collectors from 5.2×10^5 m² in
29 point A to 4.3×10^4 m² in point C. **Fig. 3** shows the dependence of the TAC of the

1 process on the total aperture area of the solar collectors for each optimal design
2 solution. Note that the energy required to drive the MEE-MVR desalination plant
3 is fulfilled using primarily solar collectors in Design A (minimum EI solution). In
4 Design B and Design C, the energy demand is covered by both the GFH and solar
5 collectors. Moreover, the GFH is required in all solutions (even in the minimum EI
6 one) as a result of the solar energy intermittency (particularly in night-time
7 operation).

8 **Fig. 4** and **Fig. 5** depict the solar energy share of each optimal design in
9 different time periods during a day in January and July, respectively. January and
10 July are the months with the lowest and largest daily solar radiation flux
11 (irradiance) in the year, correspondingly. The solar fraction as portrayed in **Fig. 4**
12 and **Fig. 5** corresponds to the amount of energy required by the boiler in the STS
13 that is covered by solar collectors. In January, all energy demands of Design A
14 (minimum EI solution) are completely fulfilled by solar collectors in time periods
15 ranging from 7 to 17h. This is due to the large area of the solar collectors used in
16 this optimal solution. As a consequence of the highest solar irradiance in July, the
17 time periods in which all energy requirements of Design A are covered by solar
18 collectors are extended from 5 to 18h. Similar behaviors are observed for Design
19 C in the winter and summer days. However, Design C only requires 17.9% of solar
20 fraction in the time period 5-6h because of its low solar irradiance (and smaller
21 solar collectors' area). Note that in remaining hours of the day, the desalination
22 systems of Design A and Design C are completely operated by using natural gas
23 in the GFH. Since the solar collector area is significantly smaller in Design B
24 (minimum TAC solution), the solar energy shares are considerably reduced in this
25 solution. For instance, 82.3% of energy requirements of Design B in January are
26 fulfilled by solar collectors in peak solar irradiance periods (11-13h). Design B only
27 achieves 100% of solar fraction share in the peak solar irradiance periods of July.
28 Therefore, better advantage can be taken from the available solar irradiance by
29 increasing the collectors' area.

1 **Fig. 6** exhibits the costs breakdown for the different optimal design
2 solutions. The TAC of the Design C (6867 kUS\$/year) is comprised by 6721
3 kUS\$/year associated with capital investment in equipment, along with 146
4 kUS\$/year related to operating (electricity, natural gas, and cooling water
5 consumption) and maintenance expenses. As the MEE-MVR desalination plant of
6 Design C is similar to that obtained in Design A, both solutions present the same
7 corresponding capital cost of investment (2603 kUS\$/year). However, the capital
8 cost of investment in the STS is decreased by 90.4% as a result of the much smaller
9 solar collectors required in Design C. The environmental impacts breakdown for
10 the different design solutions are displayed in **Fig. 7**. As expected, Design B shows
11 the highest environmental impacts related to natural gas consumption (~662k
12 ReCiPe eco-points/year). The environmental impacts of natural gas usage in
13 Design B are ~71.4% higher than those in Design A.

14 **Fig. 8** and **Fig. 9** display the thermal power share in different time periods
15 in January and July, respectively. As shown in **Fig. 8 (a)**, the energy demands of
16 the boiler in Design B are covered by both the GFH and solar collectors in the
17 time periods ranging from 7 to 17h, while the corresponding energy requirements
18 are completely fulfilled by solar collectors in Design C. A similar behaviour is
19 observed for Design B and Design C in time periods ranging from 6 to 18h of a
20 day in July (**Fig. 9 (a)** and **Fig. 9 (b)**, respectively). This is a result of the greater
21 solar collector's area required by solution C. Hence, even in the months of lower
22 solar irradiance, the energy performance of the system can be improved by
23 increasing the collectors' area. Although the latter can represent an increase in
24 the capital costs of the STS (84.7%), the natural gas consumption can be
25 significantly reduced as well as its corresponding environmental impacts (68.9%).
26 Noticeably, other alternative trade-off optimal solutions can be chosen in the
27 Pareto curve to reduce the capital costs required for solar collectors at expense
28 of small increases in environmental impacts. For that reason, the Pareto curve
29 obtained can be a useful tool for decision-makers towards the implementation of

1 cost-effective and environment-friendly desalination systems according to their
2 preferences.

3

4 **7. Conclusions**

5 A new multi-objective model is developed for the thermo-economic and
6 environmental optimization of solar-driven ZLD systems, which are particularly
7 applied to the desalination of high-salinity shale gas wastewaters. A decentralized
8 ZLD system is proposed encompassing a solar thermal-assisted Rankine cycle unit
9 coupled to a MEE-MVR desalination plant. The solar thermal system is designed
10 for multi-period operation according the daily solar irradiance throughout the
11 year. Also, the ZLD operation of the desalination plant is ensured by specifying
12 the discharge brine salinity close to salt saturation conditions. The resulting multi-
13 objective NLP model is implemented in GAMS and solved by the epsilon-
14 constraint method via the minimization of the TAC and environmental impacts.
15 The economic objective function accounts for the capital cost of investment in
16 equipment, along with maintenance and operating expenses related to utilities
17 consumption. The environmental performance is assessed by the LCA-based
18 ReCiPe methodology.

19 A case study based on Spain's weather conditions is performed to
20 demonstrate the applicability of the proposed multi-objective approach. A set of
21 trade-off Pareto solutions is obtained revealing a reduction of ~95.1% in the TAC
22 at the expense of increasing environmental impacts in 245.9%, when comparing
23 minimum economic and environmental optimal solutions. The Pareto curve also
24 shows that intermediate optimal solutions provide significant reductions in
25 environmental impacts at small increases in the total costs. The environmental
26 impacts are mainly decreased by enlarging the area of the solar parabolic trough
27 collectors, which reduces the natural gas consumption and leads to savings in
28 operating expenses. Hence, the use of solar thermal collectors to operate the

1 MEE-MVR desalination system can be not only an eco-friendly alternative but also
2 a cost-effectively solution. Thus, our comprehensive multi-objective approach
3 represents a useful tool able to identify the best alternatives that simultaneous
4 balance both environmental and economic criteria. For this reason, our multi-
5 objective model can be used to support the decision-making process towards
6 implementing more sustainable and cost-efficient solar-driven ZLD desalination
7 systems.

8

9

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4

5

1 **Nomenclature**

2 *Acronyms*

3	BPE	Boiling Point Elevation
4	CEPCI	Chemical Engineering Plant Cost Index
5	CSP	Concentrated Solar Power
6	GAMS	General Algebraic Modelling System
7	GHF	Gas-fired Heater
8	LCA	Life Cycle Assessment
9	LCI	Life Cycle Inventory
10	LCIA	Life Cycle Impact Assessment
11	MD	Membrane Distillation
12	MEE	Multiple-Effect Evaporation
13	MED	Multiple-Effect Distillation
14	MVR	Mechanical Vapor Recompression
15	MSF	Multistage Flash Distillation
16	NEA	Non-Equilibrium Allowance
17	NLP	Non-linear Programming
18	RC	Rankine Cycle
19	RO	Reverse Osmosis
20	STS	Solar Thermal System
21	ZLD	Zero-Liquid Discharge

22

23 *Roman letters*

24	A	Heat transfer area, m ²
25	BPE	Boiling point elevation, °C
26	C^{CW}	Parameter for cooling water cost, US\$/kW year
27	$C^{electricity}$	Parameter for electricity cost, US\$/kW year
28	C^{NG}	Parameter for natural gas cost, US\$/kW year
29	$CAPEX$	Capital Expenditures, kUS\$/year

1	C_p	Specific heat, kJ/kg °C
2	C_{PO}	Cost of equipment unit, kUS\$
3	CR_{\max}	Maximum compression ratio
4	EI	Total environmental impact, points/year
5	f_{ac}	Factor of annualized capital cost
6	FBM	Correction factor for the capital cost
7	f_i	Fractional interest rate per year
8	FP	Parameter for the capital cost estimation
9	G	Solar radiation flux (irradiance), kW/m ²
10	H	Specific enthalpy, kJ/kg
11	$LCIA$	Environmental impacts points, points/kW year
12	LHV	Lower heating value
13	$LMTD$	Logarithmic mean temperature difference
14	\dot{m}	Mass flowrate, kg/s
15	$OPEX$	Operational Expenses, kUS\$/year
16	P	Pressure, kPa
17	ΔP_{\min}	Minimum pressure approach, kPa
18	Q	Heat flow, kW
19	rt	Retention time in the flashing tanks, min
20	S	Salinity, g/kg
21	s	Specific entropy, kJ/kg
22	T	Temperature, °C
23	TAC	Total annualized cost, kUS\$/year
24	ΔT_{\min}	Minimum temperature approach, °C
25	U	Overall heat transfer coefficient, kW/m ² K
26	V	Volume, m ³
27	X^{salt}	Salt mass fraction
28	x	Vapor quality

1	W	Compression work, kW
2	y	Number of years
3		
4	<i>Subscripts</i>	
5	i	Evaporation effects
6	in	Inlet condition
7	out	Outlet condition
8	t	Time period
9		
10	<i>Superscript</i>	
11	amb	Ambient
12	avg	Average
13	cv	Condensate (or Distillate) vapor
14	CW	Cooling water
15	GFH	Gas-fired heater
16	IS	Isentropic
17	L	Liquid
18	mix	Mixture
19	ng	Natural gas
20	RC	Rankine Cycle
21	sat	Saturated vapor
22	SC	Solar collectors
23	STS	Solar thermal system
24	sup	Superheated vapor
25	V	Vapor
26		
27	<i>Greek letters</i>	
28	γ	Heat capacity ratio
29	η	Efficiency

1	θ	Temperatures difference, °C
2	λ	Latent heat of vaporization, kJ/kg
3	ν	Specific volume
4	ρ	Density, kg/m ³
5		
6		

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1 **Appendix. Thermodynamic Correlations**

2 The thermodynamic correlations to estimate the boiling point elevation (BPE), and
3 the fluid physical properties are presented as follows.

4

5 **A.1. Boiling Point Elevation**

6 The BPE corresponds to the raise in the temperature of boiling point triggered by
7 the salt concentration of brine. The BPE in evaporation effect i is estimated by
8 the following equation.

9

$$10 \quad BPE_i = \left(\begin{array}{l} 0.1581 + 2.769 \cdot X_i^{salt} - 0.002676 \cdot T_i^{ideal} \\ + 41.78 \sqrt{X_i^{salt}} + 0.134 \cdot X_i^{salt} \cdot T_i^{ideal} \end{array} \right) \quad \forall i \in I \quad (A.1)$$

11 Where,

$$12 \quad X_i^{salt} = 0.001 \cdot S_i^{brine} \quad \forall i \in I \quad (A.2)$$

13

14 In **Eq. (A.1)**, T_i^{ideal} is the ideal temperature ($^{\circ}\text{C}$) and X_i^{salt} the salt mass
15 fraction in the evaporation effect $i \in I$. The ideal temperature is the theoretical
16 temperature that a stream would assume if its salt concentration was equal to
17 zero. In **Eq. (A.2)**, S_i^{brine} is the brine salinity in the effect $i \in I$.

18

19 **A.2. Physical Properties of Fluids**

20 The thermodynamic properties of fluids in each evaporation effect are estimated
21 via correlations obtained from Aspen HYSYS-OLI. The process simulations have
22 been performed by using the electrolytes thermodynamic package. The
23 thermodynamic correlations for properties estimation are presented as follows.
24 They are valid for temperatures between 10°C to 120°C , and salt concentrations
25 in a range of 0 to 0.3.

26

27

1 A.2.1. Specific Enthalpy

2 The specific enthalpies of liquid and vapor states of fluids in the evaporation effect
3 i are given by the following correlations.

$$4 \quad H_i^{liquid} = -15940 + 8787 \cdot X_i^{salt} + 3.557 \cdot T_i^{boiling} \quad \forall i \in I \quad (\text{A.3})$$

$$5 \quad H_i^{vapor} = -13470 + 1.840 \cdot T_i^{boiling} \quad \forall i \in I \quad (\text{A.4})$$

6
7
8 In which, $T_i^{boiling}$ represents the boiling temperature in effect $i \in I$ given in
9 °C. To evaluate the specific enthalpies of condensate flows, we consider salt
10 concentrations equal to zero and the corresponding temperature $T_i^{condensate}$ in **Eq.**
11 **(A.3)**. The specific enthalpy of the feed salt water is also obtained by **Eq. (A.3)** by
12 taking the appropriate salt mass fraction (X_{in}^{feed}) and temperature (T_{in}^{feed}).

13

14 A.2.2. Latent Heat of Vaporization

15 The latent heat of vaporization of the streams in the evaporation effect i is given
16 as follows.

17

$$18 \quad \lambda_i = 2502.5 - 2.3648 \cdot T_i^{sat} + 1.840 \cdot (T_{i-1}^{sat} - T_i^{sat}) \quad \forall i > 1 \quad (\text{A.5})$$

19

20 In which, T_i^{sat} indicates the temperature of the saturated vapor in effect
21 $i \in I$ expressed in °C. The saturated vapor temperature is estimated via the
22 Antoine Equation for vapor-liquid equilibrium as shown in **Eq. (A.6)**.

23

$$24 \quad \ln(P_i^{sat}) = A + \frac{B}{(T_i^{sat} + C)} \quad \forall i \in I \quad (\text{A.6})$$

25

26 In which, P_i^{sat} is the saturation pressure of streams given in kPa. Moreover,
27 A , B , and C are the Antoine parameters with values equal to 12.98437, -

1 2001.77468, and 139.61335, correspondingly. **Eq. (A.6)** can also be used to
2 estimate the ideal temperature T_i^{ideal} in evaporation effect $i \in I$. In this case, the
3 pertaining pressure of vapor (P_i^{vapor}) should be considered in **Eq. (A.6)**.

4

5 *A.2.3. Specific Heat*

6 The specific heat of the feed water in the last evaporation effect $i = I$ is given as
7 follows.

8

$$9 \quad C_{p_{in}^{feed}} = 0.001 \cdot \left[\begin{array}{l} 4206.8 - 6.6197 \cdot S_{in}^{feed} + 1.2288e^{-2} \cdot (S_{in}^{feed})^2 + \\ (-1.1262 + 5.418e^{-2} \cdot S_{in}^{feed}) \cdot T_{in}^{feed} \end{array} \right] \quad (A.7)$$

10

11 The specific heat of the condensate can be obtained by considering the
12 stream salinity equal to zero in **Eq. (A.7)**. Thus,

13

$$14 \quad C_{p_i^{condensate}} = 0.001 \cdot (4206.8 - 1.1262 \cdot T_i^{ideal}) \quad \forall i = I \quad (A.8)$$

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List of Figure Captions

Fig. 1. Schematic diagram for the solar-based zero-liquid discharge desalination system. GFH, gas-fired heater; MEE-MVR, multiple-effect evaporation with mechanical vapor recompression.

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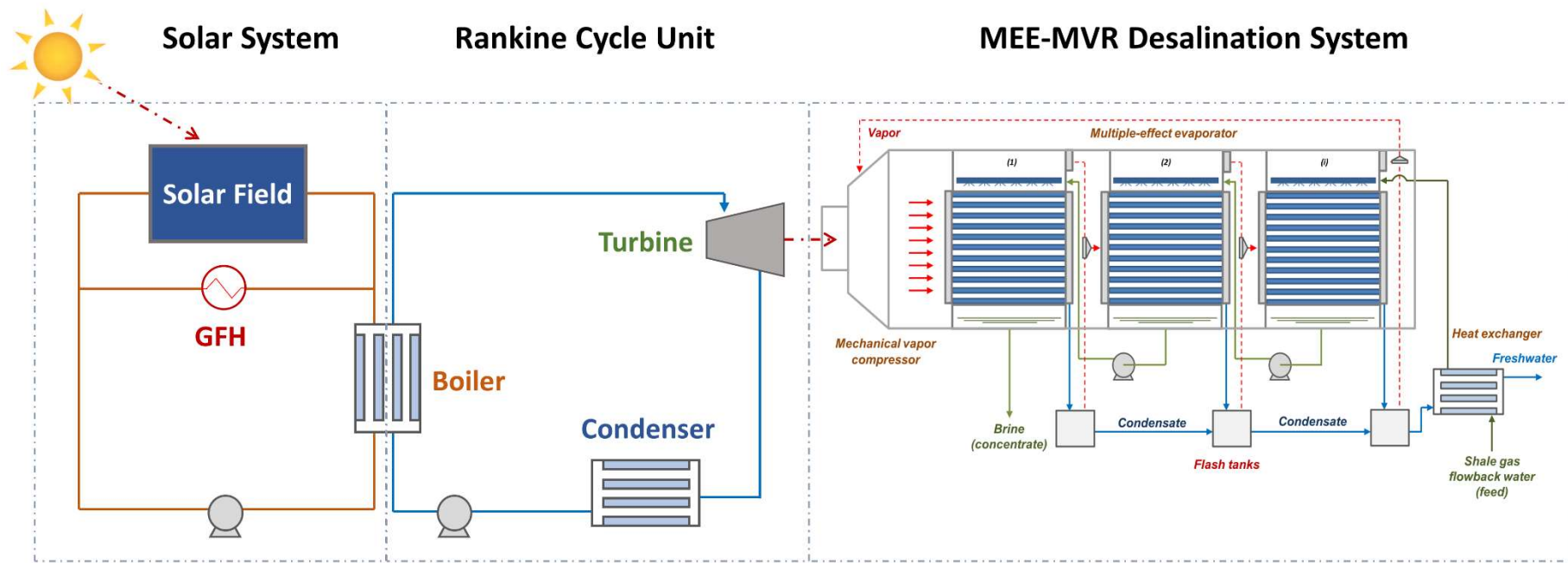


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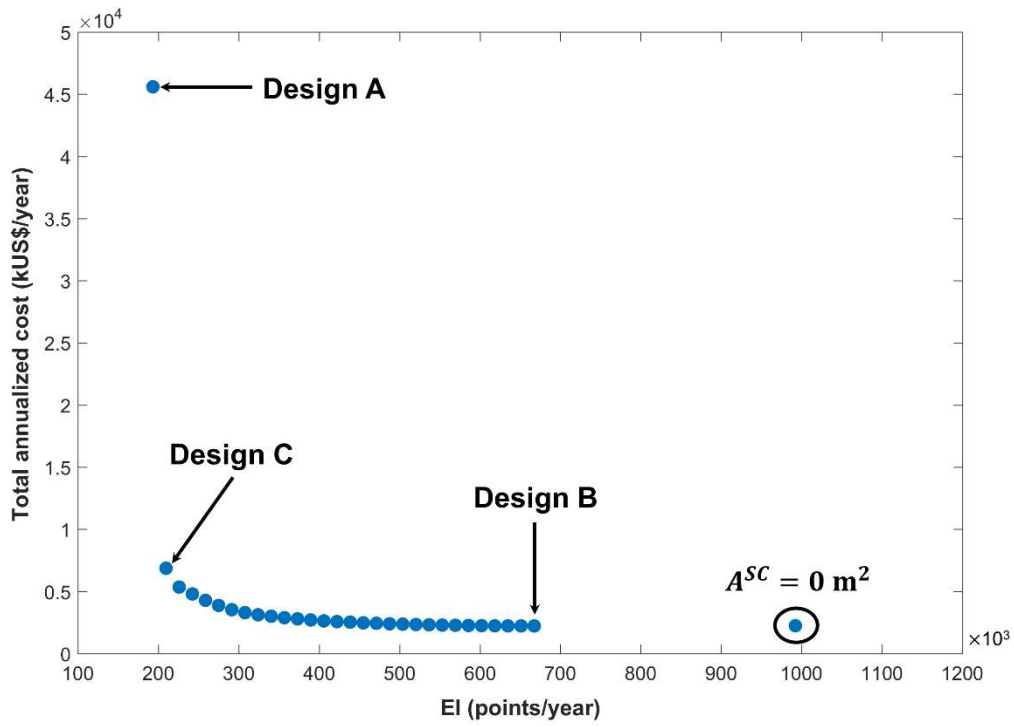


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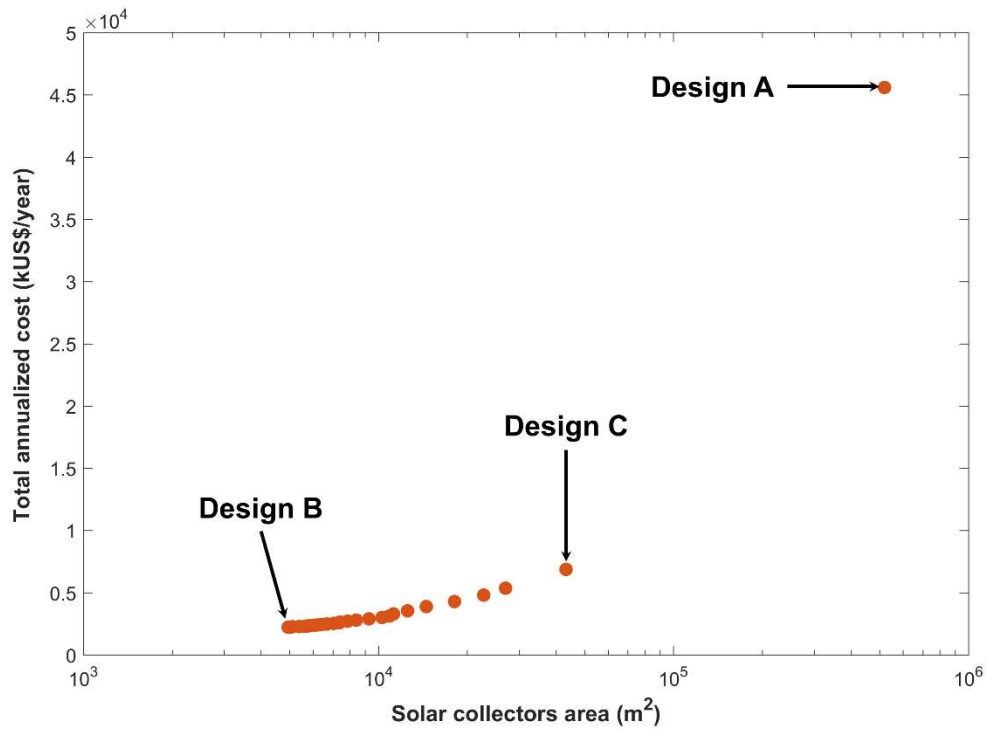


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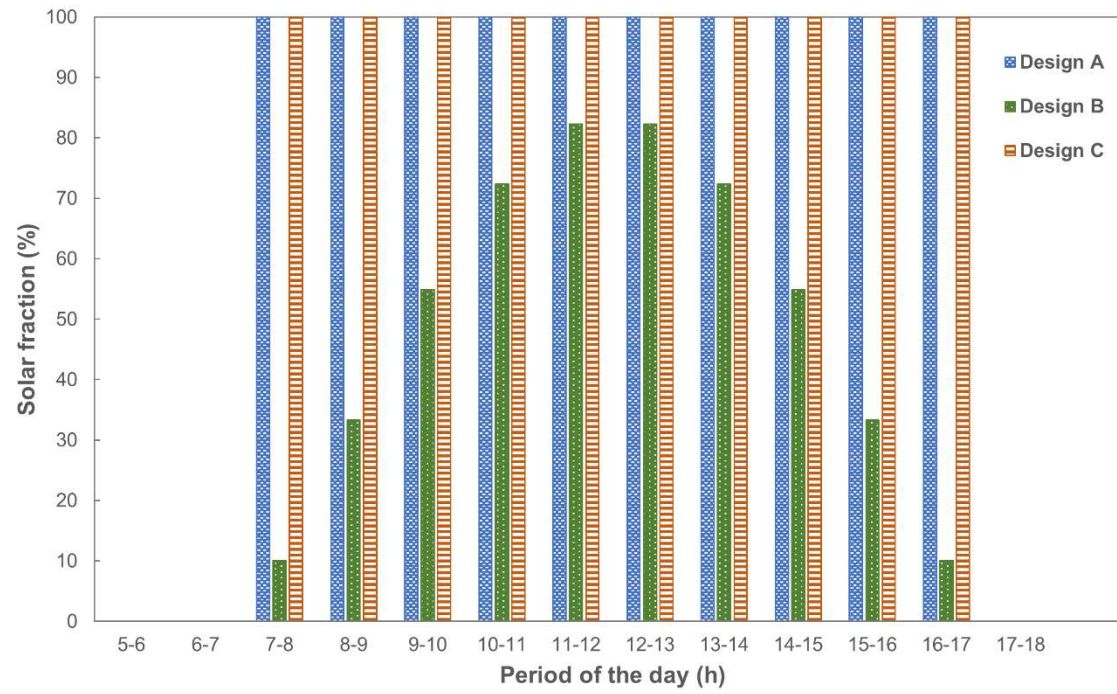


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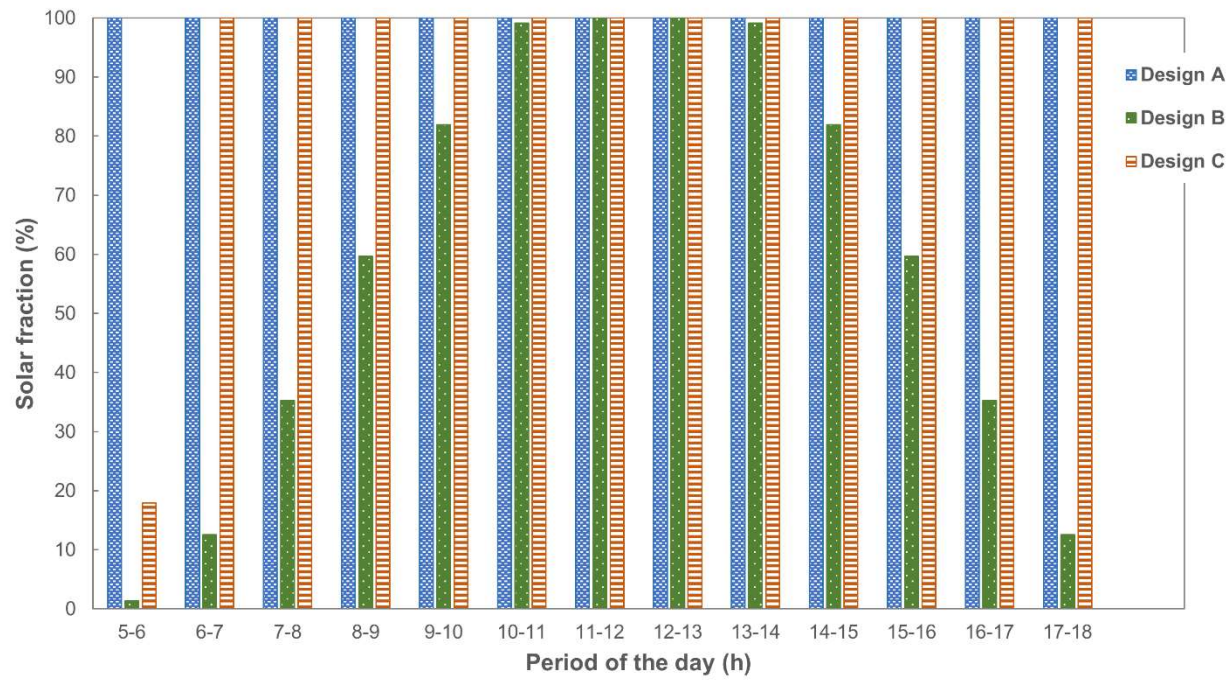


Fig. 5. Solar energy share in different time periods during a summer day in July.

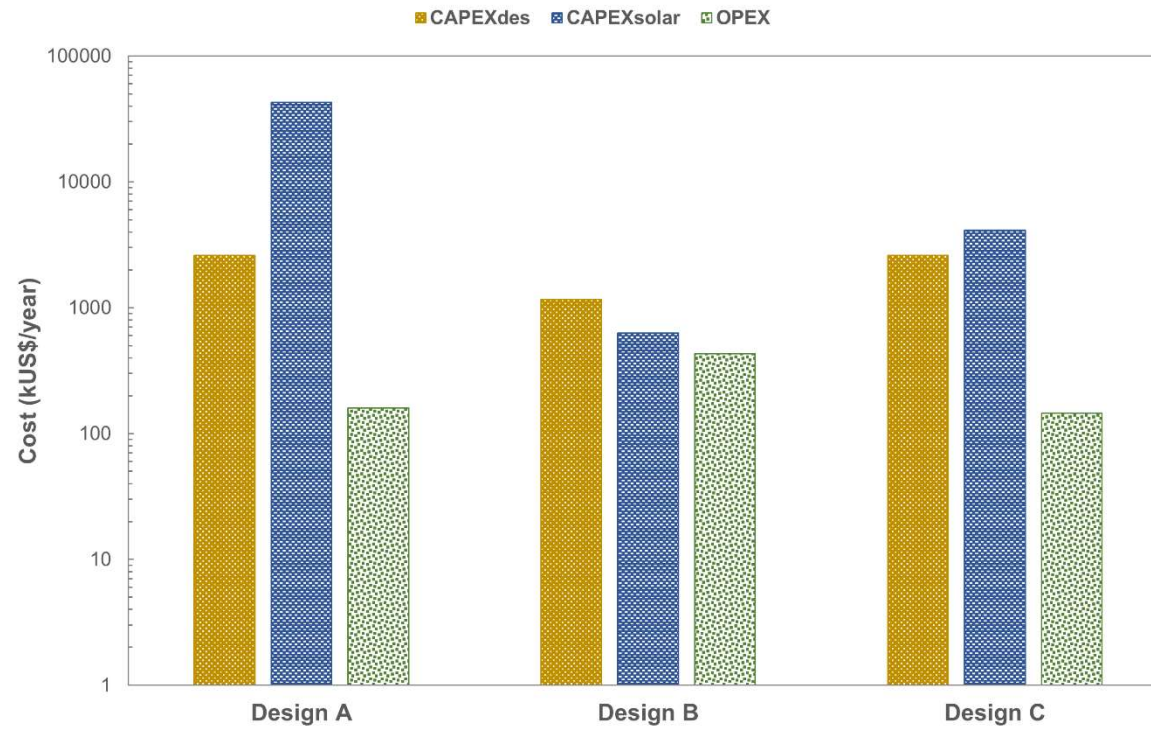


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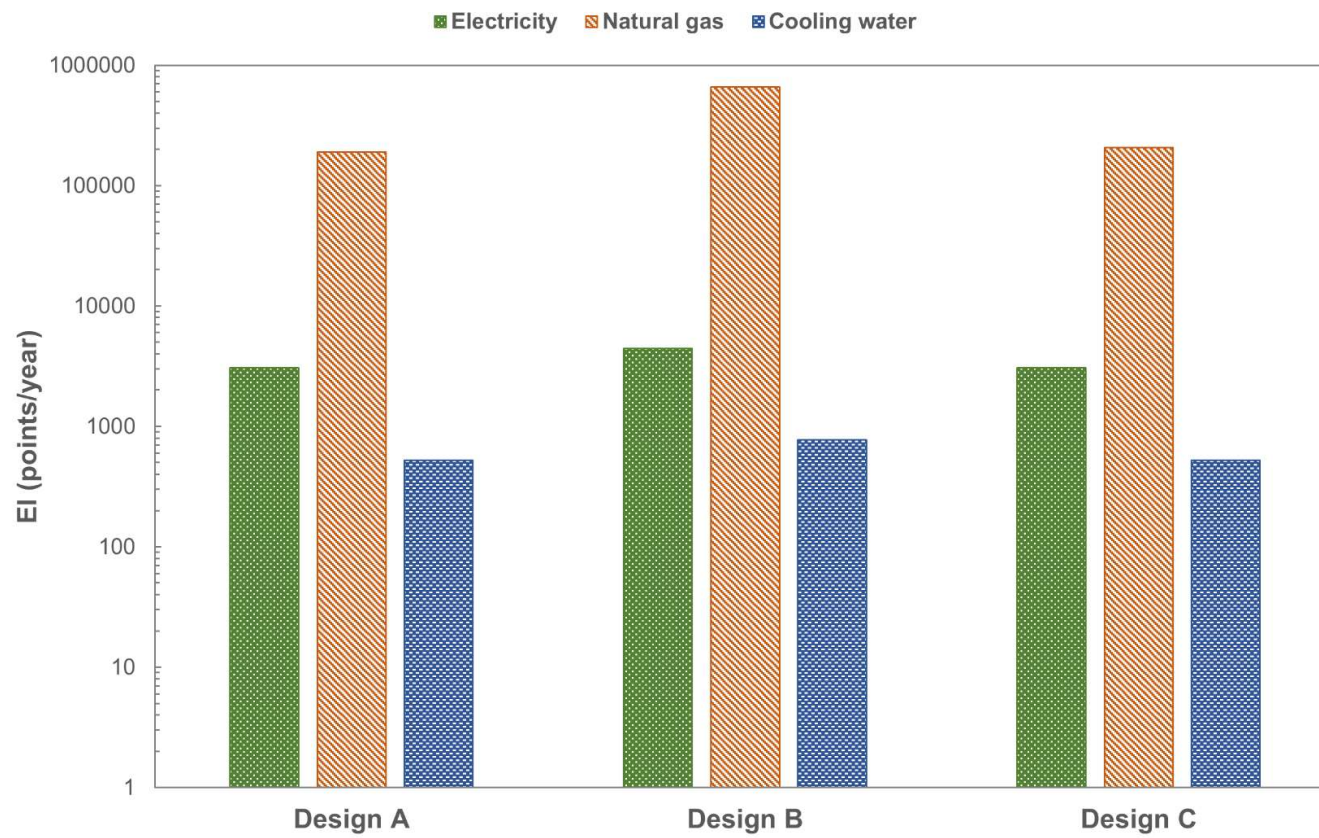


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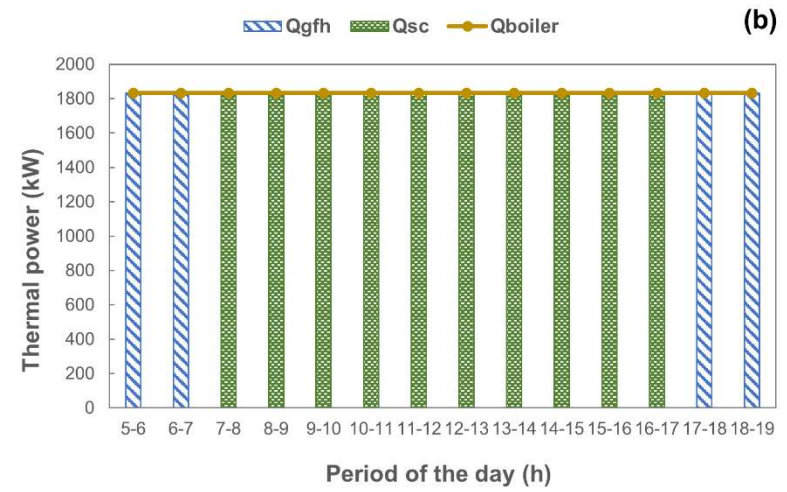
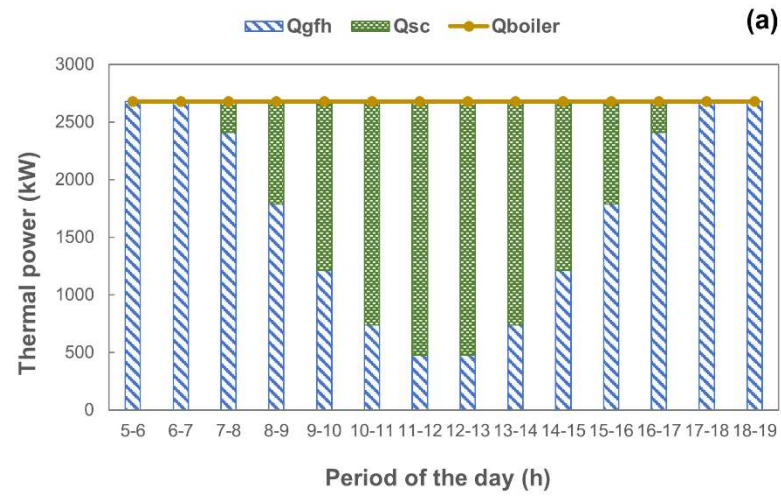


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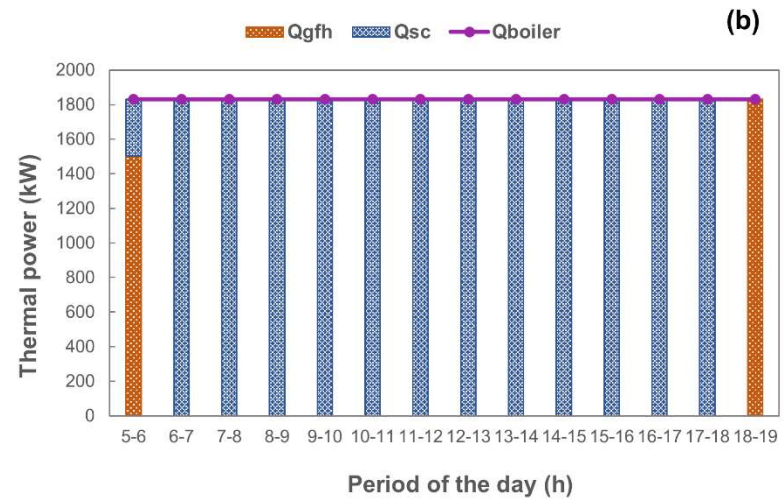
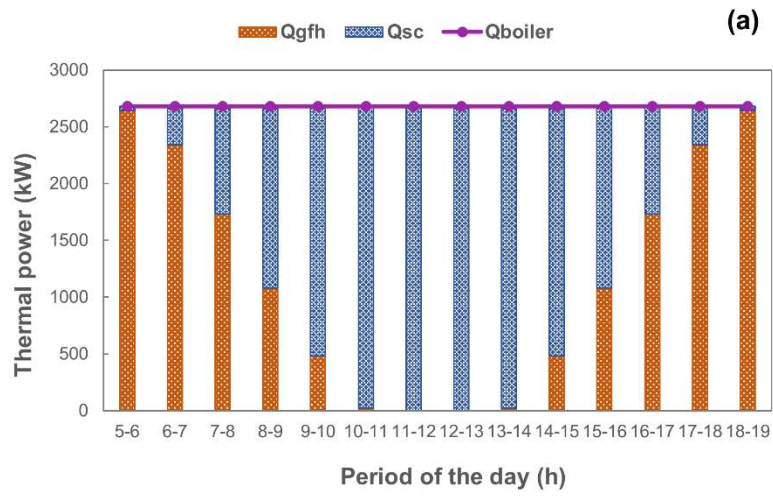


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Table 1

Parameters used in the mathematical model for the optimal design of the zero-liquid discharge MEE-MVR system.

Feed water	Mass flowrate, \dot{m}_i^{feed} (kg/s)	10.42
	Temperature, T_i^{feed} (°C)	25
	Salinity, $S_{in}^{feed_water}$ (g/kg or k ppm)	70
Mechanical vapor compressor	Isentropic efficiency, η^{IS} (%)	75
	Heat capacity ratio, γ	1.33
	Maximum compression ratio, CR_{max}	3
Process specification and operating constraints	Salinity of ZLD operation, S^{design} (g/kg or k ppm)	300
	Maximum temperature, T_i^{ideal} (°C)	100
	Maximum pressure, P_i^{sat} (kPa)	200
	Number of evaporation effects	2
Economic data	Electricity price ¹ , $C^{electricity}$ (US\$/kW year)	812.47
	Fractional interest rate per year, f_i	0.1
	Amortization period, y	10
	Working hours per year, (h)	8760

¹ Cost data obtained from Eurostat database (2020) (1st semester – 2020).

Table 2

Parameters used in the mathematical model for the optimal design of the steam Rankine cycle and solar thermal system (Salcedo et al., 2012).

Rankine cycle	Turbine isentropic efficiency, η^{IS} (%)	78
	Specific heat of water vapor, C_p (kJ/kg K)	2.7
	Inlet cooling water temperature, T_{in}^{CW} (K)	298
	Outlet cooling water temperature, T_{out}^{CW} (K)	308
Solar collectors	Collector optical efficiency, η_0 (%)	75
	Solar collector constant, a_1	4.5e-6
	Solar collector constant, a_2	0.039
	Solar collector constant, a_3	3e-4
	Specific heat of the thermal fluid (Therminol 72), C_p^{hf} (kJ/kg K)	2.528
Gas-fired heater	Efficiency, η^{GFH} (%)	75
	Lower heating value of natural gas, LHV (kJ/kg)	47100
Pump	RC pump efficiency, η^{RC_pump} (%)	60
	Specific volume of working fluid, ν (m ³ /kg)	1.2e-3
Economic data	Natural gas price ¹ , C^{NG} (US\$/kW year)	277.03
	Fractional interest rate per year, fi	0.1
	Amortization period, y	10
	Working hours per year, (h)	8760

¹ Cost data obtained from Eurostat database (2020) (1st semester – 2020).

Table 3

Daily solar radiation flux (irradiance)¹ throughout the year (Salcedo et al., 2012).

Month	5-6	6-7	7-8	8-9	9-10	10-11	11-12	12-13	13-14	14-15	15-16	16-17	17-18	18-19
<i>January</i>	0.00	0.00	92.78	260.28	416.67	543.89	615.28	615.28	543.89	416.67	260.28	92.78	0.00	0.00
<i>February</i>	0.00	0.00	155.83	322.22	488.06	621.67	696.39	696.39	621.67	488.06	322.22	155.83	0.00	0.00
<i>March</i>	0.00	57.50	211.11	387.78	559.17	695.56	771.39	771.39	695.56	559.17	387.78	211.11	57.50	0.00
<i>April</i>	3.61	90.00	253.89	433.89	604.44	743.33	816.94	816.94	743.33	604.44	433.89	253.89	90.00	3.61
<i>May</i>	25.28	106.94	272.22	448.06	615.00	741.67	811.11	811.11	741.67	615.00	448.06	272.22	106.94	25.28
<i>June</i>	34.17	112.50	276.94	452.22	611.39	733.61	800.28	800.28	733.61	611.39	452.22	276.94	112.50	34.17
<i>July</i>	30.00	109.44	274.44	450.83	611.94	736.11	803.89	803.89	736.11	611.94	450.83	274.44	109.44	30.00
<i>August</i>	13.89	97.22	261.11	438.61	609.44	740.00	811.39	811.39	740.00	609.44	438.61	261.11	97.22	13.89
<i>September</i>	0.00	70.83	226.67	402.78	571.94	705.83	785.56	785.56	705.83	571.94	402.78	226.67	70.83	0.00
<i>October</i>	0.00	0.00	173.61	341.11	506.67	639.17	713.06	713.06	639.17	506.67	341.11	173.61	0.00	0.00
<i>November</i>	0.00	0.00	112.50	270.56	425.56	551.39	621.94	621.94	551.39	425.56	270.56	112.50	0.00	0.00
<i>December</i>	0.00	0.00	70.28	235.83	386.67	510.00	579.44	579.44	510.00	386.67	235.83	70.28	0.00	0.00

¹ Irradiance values given in kW/m²

Table 4

Environmental impact points of the utilities.

Utility	Process	Total ReCiPe eco-points (points/kW year)
Electricity	Electricity, production mix ES	949.32
Natural gas	Natural gas, burned in industrial furnace > 100 kW	454.49
Cooling water	Tap water production, underground water with chemical treatment	0.396