



Research Paper

Carbon-neutral tri- and multi-generation plants with CO₂ capture unit integrated modified gas turbine, recuperative steam Rankine, absorption chiller, and MED: life cycle assessment and multi-scenario chameleon swarm optimization with XGBoost modeling

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ABSTRACT

The decarbonization of fossil fuel-powered systems remains a critical challenge due to the energy penalties and economic burdens associated with conventional CO₂ capture technologies. This issue is particularly pronounced in tri- and multi-generation systems, where integrating carbon capture without compromising efficiency and profitability requires advanced system-level solutions. Addressing this challenge is essential to enable reliable low-carbon energy supply while meeting increasing demands for electricity, heating, cooling, and freshwater. This study proposes and systematically examines advanced carbon-neutral tri- and multi-generation energy systems featuring deep thermal integration and alternative heat supply strategies for CO₂ capture. Two integration scenarios are investigated: a methane-fueled tri-generation system incorporating a MEA-based CO₂ capture unit (System I), and an extended multi-generation configuration supported by geothermal energy to drive CO₂ capture and desalination (System II). Comprehensive thermo-enviro-economic assessments, gate-to-gate life cycle assessment, and data-driven multi-objective optimization using XGBoost surrogate modeling and advanced metaheuristic algorithms are employed. System I achieves 54.00% exergy efficiency and 98.78% CO₂ removal, reducing emissions to 21.47 kg/h, while System II further enhances performance, attaining 54.51% exergy efficiency, reducing specific GWP to 0.0179 kg/kWh, and increasing NPV to 14.07 M\$. Optimized operation yields exergy efficiency up to 55.28% with minimal economic and environmental impact. The proposed systems provide a scalable and economically viable pathway for deploying carbon-neutral multi-generation plants in industrial and urban energy hubs, supporting long-term decarbonization and sustainable energy transition strategies.

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1. Introduction

A major issue in today's quickly changing world is the growing demand for dependable and sustainable energy, which is being driven by urbanization, population increase, industrial development, and technological advancement [1,2]. Despite continued dominance of traditional fossil fuel-based energy systems, they are becoming more widely acknowledged as unsustainable because of their finite supplies and their detrimental effects on the environment, especially with regard to greenhouse gas emissions, air pollution, and climate change [3,4]. Alternative solutions such as tri-generation [5] and multi-generation [6] systems that not only satisfy the growing need for energy but also tackle issues of sustainability and efficiency are now desperately needed. In contrast to conventional energy plants that usually concentrate on a single form of output, tri-generation systems are designed to produce valuable outcomes. This integrated approach significantly increases energy utilization efficiency, often reaching values above 60%, compared to less than 40% in conventional single-output systems [7]. Tri-generation systems are advantageous economically and environmentally because they minimize energy losses, reduce fuel consumption, and lower operating costs by capturing and reusing waste heat [8,9]. Additionally, these systems can be flexibly powered by natural gas [10], biomass [11], or renewable energy sources [12], increasing their adaptability to a variety of applications, from hospitals, universities, and urban residential districts.

Natural gas power plants rank among the most employed tri-generation methods in which the process start with the gas turbine arrangements. In these systems, combustion of the natural gas generates high-temperature and high-pressure gases whose rapid expansion makes the turbine blades move and turns thermal energy into mechanical movement, which the generator converts into electricity. In order to enhance the overall efficiency of system, one major benefit of such plants is the capability to recover the released heat to a great extent through multiple heat-recovery processes. Lei et al. [13] proposed a power plant powered by natural gas integrated with different energy module to reduce regeneration energy demand, which realized an 18.03% saving on regeneration energy usage, reduced exergy destruction by 24.23 MW, and increased net power efficiency to 51.40%. Moreover, Yan et al. [14] investigated a tri-generation scheme on the basis of natural gas-based combined cycles accompanied by effective production 111 MW power and 175.6 kg/s cooling. Aghaei and Saray [15] proposed a combined tri-generation system with gas turbine mover. Results showed that while the base design favors a high compressor pressure ratio (14.79) and the inclusion of an air pre-heater, optimized scenarios converge to lower pressure ratios of 6. Li et al. [16] upgraded gas turbine-driven energy system with reduced emissions, which achieved an 8% cost reduction, 1.2% CO₂ avoidance, and 5% exergy efficiency augmentation in optimized configuration.

Furthermore, by integrating the power generation process with the heat-recovery process, natural gas plants make the reliable and efficient tri-generation with relatively environmentally friendlier than many other fossil fuel-based technologies and minimized energy losses [17,18]. In such systems, the excess thermal energy emanating from primary processes, in the flue gases of a gas turbine, can be captured efficiently and used in a Rankine cycle to recover low-temperature waste heat into added electricity, thus raising power output without the necessity for additional fuel combustion [19,20]. Beyond electricity generation, the recovered heat can be effectively applied to industrial processes or building heating, maximizing energy utilization and reducing dependence on external heat sources [21]. Also, directing part of this recovered heat into refrigeration units allows for the production of chilled water, serving air conditioning and refrigeration demands [22,23]. Bi et al. [24] demonstrated that hybrid air-water heat-sink integration significantly improves long-term thermal management while reducing system size, underscoring the value of deep thermal integration in advanced energy systems. Li et al. [25] showed that tightly integrated

micro-combustion and thermoelectric cooling, heating, and power systems can surpass battery-based power sources in energy density through system-level thermal-fluid optimization. Mi et al. [26] proved that multi-stage water injection provides markedly superior thermal mitigation of rocket exhaust plumes than single-stage injection, significantly reducing peak temperatures and high-temperature zones without compromising thrust, thereby extending component lifespan through optimized staged cooling design.

Despite these advantages, the environmental performance of natural gas-based tri-generation systems remains constrained by non-negligible CO₂ emissions, which limits their alignment with carbon-neutral energy strategies. To mitigate this limitation, recent research has explored the integration of carbon capture technologies into energy systems. For instance, Gimelli et al. [27] integrated ammonia–water absorption cycles in a hospital-based tri-generation configuration for power and cooling with battery-supported natural gas engines. Despite the relatively high upfront cost, their analysis demonstrated significant energy and environmental benefits, including a 19.88% reduction in fossil primary energy consumption and a 23.99% cut in CO₂ emissions. Similarly, Abdoos et al. [28] integrated a Rankine cycle (steam) into tri-generation system, which successfully met regional energy demands by delivering 41,103 kW of electricity, 111,000 kW of heating, and 1100 kW of cooling. Complementing these efforts, Yang et al. [29] introduced a dual-fuel system employing both biomass and natural gas for a hotel application, conducting a seasonal thermodynamic and exergo-economic analysis. Their findings indicated exergy efficiencies of 8.06% in summer and 12.23% in winter, with the gasifier identified as the primary source of exergy destruction.

Adding a decarbonization unit to a tri-generation system is a proactive way to reduce environmental impacts and increase energy efficiency at the same time. In traditional tri-generation systems, electricity, heating, and cooling are all produced from a single fuel source, but significant CO₂ emissions are often released during the process. By adding a decarbonization module, such as CO₂ capture and storage [30], chemical absorption CO₂ [31], or membrane-based CO₂ separation [32], to the system, a significant amount of the produced CO₂ during the combustion stage can be separated, stored, used, or transformed into value-added products. This integration not only reduces greenhouse gas emissions but also improves the plant's sustainability profile by aligning with global carbon-neutral targets. Fan et al. [33] investigated tri-generation system, which utilized chemical looping combustion to reduces greenhouse gas emissions. Results showed that under design conditions the system achieved 60.16% energy efficiency and 22.16% exergy efficiency with oxygen to CO₂ ratio of 0.42. Yin et al. [34] cryogenic carbon capture into energy system, offering large-scale energy storage and CO₂ reduction. The system's potential to reduce energy, exertion, and emissions demonstrated its superior performance and social benefits compared to conventional CO₂ storage systems. Liu et al. [35] proposed a tri-generation system that utilized CO₂ capture, showing outputs of 29.601 MW cooling, 4.211 MW heating, 12.036 MW net power, and a CO₂ capture rate of 7.9236 t/h at 38.39% exergy efficiency. Through multi-objective optimization, the system achieved 90.65 MW total energy output, 41.38% exergy efficiency, and a reduced cost of 18.05 \$/GJ. Yuan et al. [36] integrated a tri-generation microgrid with power-to-gas technology using a downside capturing and recycling CO₂ approach. Results showed that this integration reduced emission costs by about 55%. However, many of these investigations either treat the CO₂ capture system as a downstream add-on or focus primarily on energy-based indicators, often neglecting detailed exergy-based diagnostics and life cycle environmental impacts. Furthermore, the majority of existing studies evaluate system performance under fixed operating conditions, offering limited insight into optimal design and operational trade-offs.

Parallel to system integration efforts, optimization techniques have increasingly been employed to enhance the performance of tri- and multi-generation systems. Early studies predominantly relied on single-

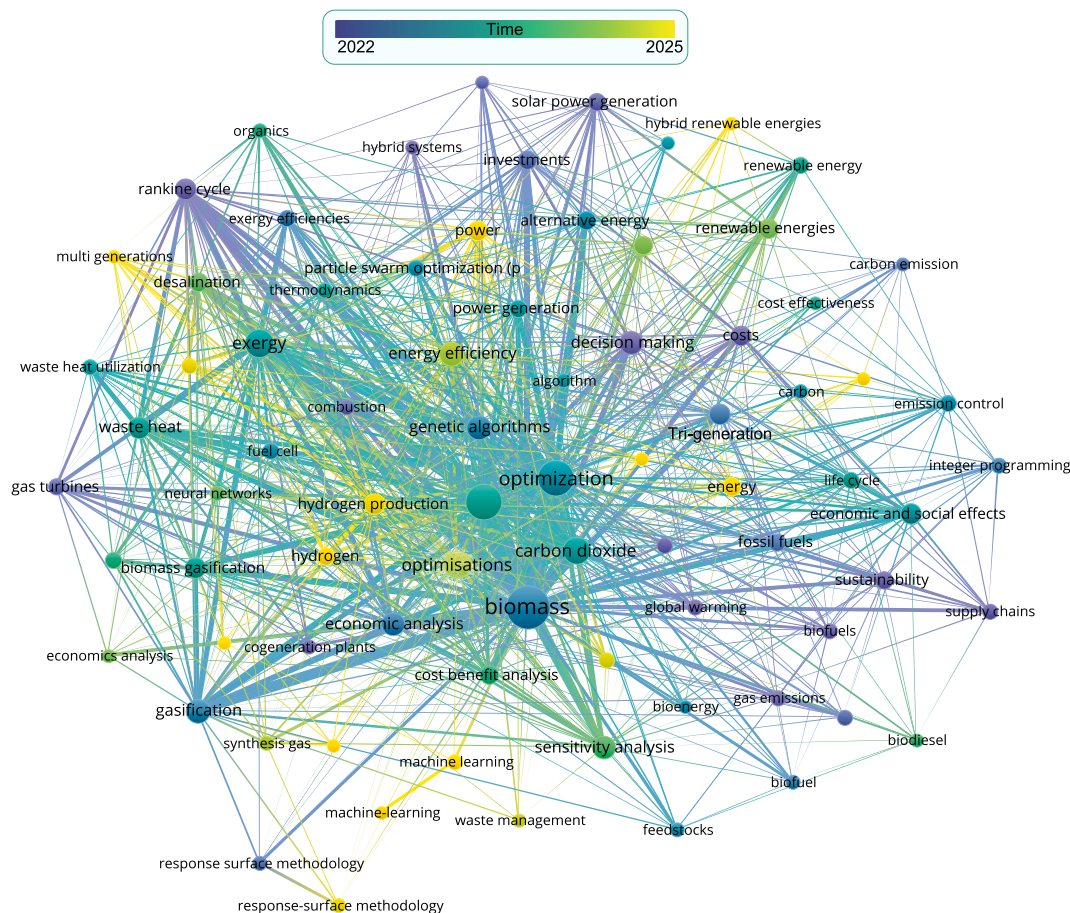


Fig. 1. Comparative literature review, highlighting the distinct methodological scope of the present study.

objective optimization approaches aimed at maximizing efficiency or minimizing cost [37,38]. More recent works have adopted multi-objective optimization frameworks to simultaneously address thermodynamic, economic, and environmental objectives, employing such algorithms as genetic algorithms [39], non-dominated sorting genetic algorithm II [39,40], particle swarm optimization [41], multi-objective weighted mean of vectors [42], and gray wolf optimization [43]. Although these methods have proven effective, most prior studies utilize a single optimization algorithm without comparative benchmarking, and few integrate advanced machine learning surrogates to reduce computational cost while preserving optimization accuracy.

Recent studies have also explored optimization in the context of carbon capture and low-carbon energy systems; however, these efforts typically focus on isolated subsystems or single technologies. For instance, Zhang et al. [44] investigated systematic optimization of CaO-based CO₂ adsorption and demonstrated how operating parameters influence adsorption efficiency, but their analysis was limited to material-level performance without system-level integration or multi-product energy evaluation. Similarly, Meng et al. [45] optimized wind-integrated power systems with carbon capture and energy storage under carbon pricing mechanisms, yet their framework did not address thermally integrated tri- or multi-generation architectures, renewable-assisted reboiler supply, or freshwater production.

1.1. Gap identification

A critical assessment of recent literature reveals several unresolved gaps in the development of advanced tri-generation and multi-generation energy systems. Although numerous studies have investigated gas turbine-based combined cooling, heating, and power (CCHP)

systems, most existing works treat key subsystems in a largely sequential or decoupled manner, rather than through deep thermodynamic integration.

First, fully integrated tri-generation systems with explicit thermal coupling to CO₂ chemical absorption units remain limited. In many reported configurations, carbon capture is either excluded or treated as an external add-on, with insufficient attention to the interaction between power generation, waste heat recovery, cooling production, and solvent regeneration. Consequently, the potential for cascading heat utilization and system-level efficiency enhancement is not fully realized.

Second, although energy and exergy analyses are commonly reported, comprehensive multi-dimensional assessment frameworks that simultaneously integrate energy, exergy, exergo-economic, exergo-environmental, and life cycle assessment (LCA) remain scarce, despite their importance for realistic sustainability evaluation. The absence of such holistic approaches limits the ability to draw robust conclusions regarding the true sustainability and competitiveness of integrated carbon-neutral systems.

Third, the application of hybrid data-driven optimization frameworks, which combine machine learning models with advanced multi-objective metaheuristics and objective-weighting techniques, has not been sufficiently explored in the context of carbon-neutral tri-generation systems.

Finally, the comparative utilization of an alternative low-carbon heat source for CO₂ capture regeneration has received little attention. In particular, the choice between internally recovered waste heat (e.g., from steam Rankine cycle) and externally supplied renewable heat (e.g., geothermal energy) has not been systematically evaluated within a unified multi-generation platform. This gap is critical, as the source of reboiler heat strongly influences system flexibility, carbon intensity, and

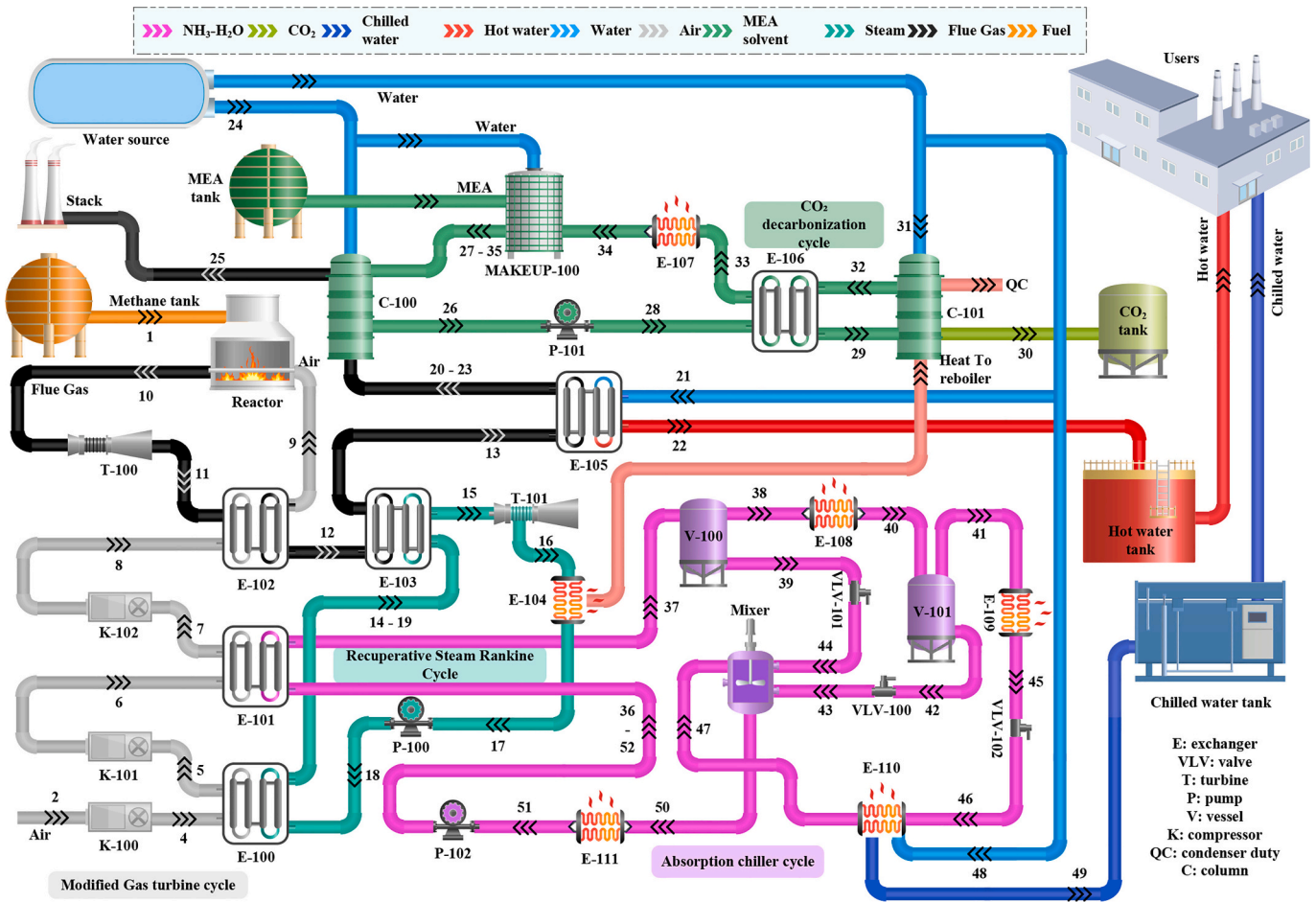


Fig. 2. The configuration of methane-fueled tri-generation system integrated with decarbonization unit for CO₂ capture (first scenario).

operational robustness.

Fig. 1 presents a comparative overview of previously published tri- and multi-generation studies, clearly illustrating the key methodological gaps that motivate the proposed carbon-neutral framework.

1.2. Novelty and contributions

To address the above-mentioned gaps, the present study proposes advanced carbon-neutral tri- and multi-generation energy systems with a particular focus on system-level thermal integration and comparative utilization of alternative heat sources for CO₂ capture, rather than the introduction of isolated components. Two distinct integration scenarios are developed and evaluated within a unified modeling framework.

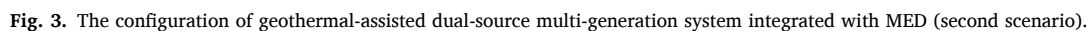
In the first scenario (**System I: tri-generation**), a CO₂ chemical absorption unit is directly integrated into a modified gas turbine-based energy conversion architecture. The system also incorporates a recuperative steam Rankine cycle, a boiler, and an absorption chiller to maximize cascade utilization of fuel energy while achieving near-zero carbon emissions. Hence, it is a design of a deeply integrated configuration in which multiple internal energy streams are synergistically coupled. The intercooler heat released during multi-stage air compression is recovered and valorized to drive an ammonia–water (NH₃–H₂O) absorption chiller, enabling cooling production without additional fuel consumption. The compressed air subsequently supports methane combustion and power generation in a modified gas turbine. High-temperature exhaust gases are then recovered in a steam Rankine cycle, producing additional power and hot water. A key novelty of this scenario is the direct thermal coupling between the steam Rankine cycle and the Mono-Ethanol-Amine (MEA)-based CO₂ capture unit, whereby a

dedicated heat stream supplies the reboiler regeneration duty. This Rankine–carbon capture integration significantly reduces waste heat rejection and enhances overall energy utilization.

In the second scenario (**System II: multi-generation**), a fundamentally different integration pathway is introduced by supplying the CO₂ capture reboiler heat using geothermal energy instead of recovered exhaust heat. This approach decouples carbon capture from the combustion-based heat recovery loop, improves operational flexibility, and substantially reduces the carbon intensity of solvent regeneration. Moreover, the remaining geothermal thermal potential is further exploited for operating multi-effect desalination (MED) unit, extending geothermal utilization beyond conventional electricity, cooling, heating applications and forming an additional co-generation pathway.

A further distinguishing outcome of the proposed framework is the achievement of an exceptionally high CO₂ removal efficiency of 98.78% in the base configuration. This performance is primarily attributed to improved absorption conditions in the MEA-based unit, including reduced solvent viscosity through controlled water addition and the availability of stable and sufficient regeneration heat. Achieving such a high capture efficiency within a tightly integrated multi-generation system represents a notable advancement over conventional configurations. Therefore, the unique contributions of this study can be summarized as follows:

- Recovery and valorization of air-compression intercooler heat for absorption cooling without external energy input.
- Cascaded integration of a modified gas turbine and steam Rankine cycle for simultaneous power and heat production.



- Integration of Extreme Gradient Boosting (XGBoost) as a surrogate modeling tool to enhance optimization efficiency and robustness, coupled with Shannon entropy for objective weighting.
- Detailed parametric and sensitivity analyses to identify critical design variables governing system performance, thereby improving practical relevance and design insight.

All in all, these features move beyond incremental performance enhancement and establish a system-level, scenario-based integration framework for the design and optimization of next-generation carbon-neutral tri- and multi-generation systems, directly supporting sustainable energy transition and long-term decarbonization objectives.

2.1. Description of System I

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Table 1

Main operating parameters and characteristics of the proposed carbon-neutral systems [49,51–57].

Parameter	Value
Modified gas turbine cycle	
Air to burner (kg/s)	4.5
Fuel type	Methane
Fuel rate (kg/s)	0.2
The outlet pressure of K-100 (kPa)	400
The outlet pressure of K-101 (kPa)	1300
The outlet pressure of K-102 (kPa)	5000
The outlet pressure of T-100 (kPa)	105
The temperature at stream 9 (°C)	300
Recuperative steam Rankine cycle	
The temperature at stream 15 (°C)	355
The outlet pressure of T-101 (kPa)	230
The inlet pressure of T-100 (kPa)	8000
The outlet pressure of P-100 (kPa)	8000
Decarbonization unit	
Solvent type	MEA
Solvent mass fraction (%wt)	30
P-101 outlet pressure (kPa)	190
The temperature at Stream 29 (°C)	105
The temperature at C-101 condenser (°C)	35
C-101 reflux ratio	0.27
The temperature at stream 34 (°C)	35
Absorption chiller	
The temperature at stream 37 (°C)	140
The temperature at stream 40 (°C)	35
The temperature at stream 45 (°C)	35
The temperature at stream 47 (°C)	35
The outlet pressure of VLV-102 (kPa)	350
The outlet pressure of P-102 (kPa)	1200
Desalination unit	
Sea water temperature (°C)	25
Sea water pressure (kPa)	101.3
Fresh water temperature (°C)	35
Overall system	
Dead state temperature (°C)	25
Dead state pressure (kPa)	101.3
Chilled water temperature (°C)	8
Hot water temperature (°C)	80
Fuel gas pressure from refinery (kPa)	5000
Geothermal inlet temperature (°C)	220
Geothermal inlet pressure (kPa)	2318

with nearly zero-carbon emission, the operational procedure of which is depicted in Fig. 2. The configuration integrates a modified gas turbine cycle, a recuperative steam Rankine cycle, an absorption chiller cycle, and a CO₂ decarbonization unit, ensuring simultaneous production of power, heating, and cooling while minimizing carbon emissions.

• Modified gas turbine cycle

In the start of the procedure, the compression of combustion air in three sequential compressors, K-100, K-101, and K-102 is occurred. During the compression, the compressed air transfers its heat into steam Rankine and absorption chiller using E-100 and E-101 for reaching the favorable condition for combustion. The compressed air, before entering the gas combustion reactor, undergoes preheating in E-102 heat exchanger. This arrangement enhances combustion efficiency by supplying preheated air to the reactor. Within the combustion chamber, methane reacts with the oxidant, producing high-temperature flue gases that drive the main turbine T-100 to generate electrical power. The high-enthalpy flue gases exiting T-100 are directed through heat exchanger E-

102, into the boiler and steam Rankine where they recover heat energy from flue gases for improving efficiency.

• Boiler and steam Rankine cycle

In the boiler, the thermal energy of flue gases is utilized by E-105 to produce hot water, while in Rankine cycle the entering flue gases into the steam generator is utilized to generation the steam with much pressure. Then, this steam is expanded in T-101 turbine for generating additional electricity. The exhaust steam from T-101 is condensed in heat exchanger E-104, and the released heat is used to provide the reboiler duty for CO₂ stripping. The closed-loop Rankine cycle is maintained by the circulation of condensate through pump P-100, while recuperator E-100 ensures recovery of thermal energy to maximize cycle efficiency.

• Absorption chiller cycle

Parallel to the power and heating functions, an absorption chiller cycle is integrated to provide cooling. In this subsystem, the operation fluid is evaporated in the vapor generator of E-101, and liquid–vapor separation is occurred in vessel V-100. To further purify and enrich the vapor phase, partial condensation in E-108 and subsequent separation in V-101 vessel are performed. Then, the purified vapor is condensed in E-109 and expanded through valve VLV-102, resulting in a significant temperature drop. This cold refrigerant stream is employed in the evaporator of E-110 for producing chilled water for refrigeration or air-conditioning purposes. The refrigerant exiting E-110 is recombined with liquid streams from V-100 and V-101 via control valves VLV-100 and VLV-101 in a mixing process, followed by condensation in E-111. In this process, the Pump P-102 repressurizes the refrigerant for completing the cycle.

• CO₂ decarbonization cycle

In order to manage environmental issues, the system incorporates a decarbonization unit using a MEA-based absorption technology. In this process, the flue gas and 30 wt% MEA solvent streams are drawn into the C-100 absorption tower. In the absorber, the CO₂ is chemically absorbed into the solvent to form a CO₂-rich liquid. In this process, an attempt is made by the introduction of water from the top-most stage to reduce the loss of the solvent. The treated flue gas, devoid of CO₂, is drawn off of absorber, whereas the pressurized CO₂-rich solvent is preheated and routed to the C-101 stripper column. In the stripper, reboiler heat from the Rankine cycle delivers the required energy to desorb the CO₂ from the solvent. The stream of CO₂ is discharged from the stripper, whereas the condensed water is partially eliminated. The MEA solvent after cooling through the network of E-106 and E-107 exchangers of heat is circulated back into the absorber tower after being restored in the Make-up-100 tank. This closed-cycle solvent management approach enables both efficient CO₂ capture and prevention of the degradation of the solvent.

2.2. Description of System II

The second scenario introduces a dual-source multi-generation configuration by integrating a renewable geothermal energy source into the primary natural gas-based system. In this modified architecture (Fig. 3), geothermal heat replaces waste-heat-driven regeneration by directly supplying the reboiler duty of the MEA-based CO₂ capture unit via heat exchanger E-112. This decouples carbon capture from combustion-related heat recovery, enhances operational flexibility, and significantly reduces the carbon intensity of the regeneration process.

Beyond CO₂ capture, the residual geothermal thermal potential is cascaded to an MED subsystem, enabling the simultaneous production of freshwater and domestic hot water (DHW). This addition expands the

Table 2

Properties of the main new integrated combined cycle streams.

Stream	<i>T</i> (°C)	<i>P</i> (kPa)	<i>m</i> (kg/s)	<i>h</i> (kJ/kg)	<i>s</i> (kJ/(kg·°C))
1	35	5000	0.2	−4699	9.369
2	25	101.3	4.5	−0.2836	5.258
4	181.1	400	4.5	159.9	5.294
5	55	400	4.5	29.49	4.958
6	197.6	1300	4.5	176.5	4.989
7	40	1300	4.5	11.94	4.564
8	200.5	5000	4.5	176.9	4.599
9	300	5000	4.5	284.6	4.806
10	1855	5000	4.7	72.49	7.043
11	772	105	4.7	−1437	7.215
12	691.1	105	4.7	−1540	7.112
13	143.3	105	4.7	−2197	6.114
14	133.3	8000	1.251	−15,410	4.324
15	355	8000	1.251	−12,940	8.882
16	124.6	230	1.251	−13,540	9.049
17	25	230	1.251	−15,890	2.981
18	25.68	8000	1.251	−15,880	2.985
19	133.3	8000	1.251	−15,410	4.324
20	54.66	105	4.7	−2296	5.847
21	25	101.3	1.79	−15,890	2.981
22	85	101.3	1.79	−15,630	3.775
23	54.66	105	4.7	−2295	0.116
24	25	105	0.3253	−15,860	−9.043
25	60.06	105	4.267	−1732	0.005822
26	59.67	105	9.231	−12,180	−8.019
27	35	105	8.473	−12,260	−8.446
28	59.69	190	9.231	−12,180	−8.019
29	105	190	9.231	−12,010	−7.535
30	34.99	190	0.5509	−8990	−0.03627
31	34.99	190	0.2084	−15,800	−8.89
32	121.1	190	8.472	−11,950	−7.549
33	70.82	190	8.472	−12,130	−8.051
34	35	105	8.472	−12,260	−8.447
35	35	105	8.472	−12,270	−8.447
36	26.25	1200	0.5434	−10,240	3.845
37	140	1200	0.5434	−8875	7.546
38	140	1200	0.3101	−5386	9.634
39	140	1200	0.2333	−13,510	4.772
40	60	1200	0.3101	−6671	6.223
41	60	1200	0.1203	−2704	8.988
42	60	1200	0.1898	−9187	4.47
43	24.43	350	0.1898	−9187	4.512
44	104	350	0.2333	−13,510	4.805
45	28	1200	0.1203	−3980	4.82
46	−4.879	350	0.1203	−3980	4.859
47	11	350	0.1203	−2809	9.212
48	25	101.3	1.921	−15,890	2.981
49	8	101.3	1.921	−15,960	2.728
50	61.09	350	0.5434	−9632	5.777
51	26.13	350	0.5434	−10,240	3.844
52	26.25	1200	0.5434	−10,240	3.845

system from a conventional trigeneration platform to a multi-generation system without additional fossil fuel consumption. Owing to the increased thermal input from geothermal energy, heat exchangers E-105 and E-104 deliver higher hot water outputs compared to the first scenario, resulting in improved thermal performance and resource utilization.

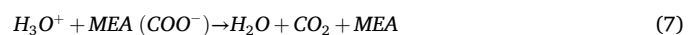
Overall, the second scenario demonstrates the effective valorization of renewable geothermal heat for both carbon capture and desalination, leading to enhanced hot water production, reduced environmental impact, and improved overall system efficiency relative to the base configuration.

2.3. System simulation

In this study, Aspen HYSYS is employed to simulate both tri- and multi-generation systems due to its capability to rigorously model complex, chemically reactive, and thermally integrated process configurations. The suggested systems involve methane–air combustion, multi-stage compression with intercooling, heat-exchanger networks,

steam Rankine cycles, absorption chiller, and MEA-based CO₂ capture and regeneration, all of which are supported by validated unit-operation models and advanced thermodynamic packages within Aspen HYSYS. This software further enables consistent mass and energy coupling across subsystems, which is essential for assessing the deep thermal integration adopted in both scenarios. Accordingly, it was chosen to ensure simulation accuracy, numerical robustness, and industrial relevance. To this end, in the first step, chemical components are selected from the Aspen library and added to the component list. Since the power plant and the decarbonization section operate with different working fluids, two separate component lists are created. The complete set of materials used in the process is summarized in Table 1.

During the second step, proper thermodynamic models is specified to precisely represent the different physiochemical regimes of the integrated system. The Peng–Robinson equation of state [46] is used for the power plant part and heat-recovery sections due to its suitability for high-temperature gas mixtures and combustion products commonly encountered in power-generation processes. For the MEA-based CO₂ chemical absorption unit, the Acid Gas–Chemical Solvents property package is employed due to its proven capability to model reactive acid gas absorption, solvent speciation, and regeneration behavior [47–49]. Both the C-100 absorption and the C-101 stripping towers are simulated as packed columns using IMTP packing, which comprised 17 and 10 equilibrium stages, correspondingly. The absorption reactions involving chemicals are automatically sorted into the equilibrium and kinetics sets within Aspen HYSYS and implemented in the flowsheet [49]. Within the absorber, the ternary system reactions of CO₂–MEA–H₂O take place according to Eqs. (1)–(7), which occur in the stripper at elevated temperatures to enable solvent regeneration [47–50]:



Other assumptions for the thermodynamic modeling and analysis of the suggested tri- and multi-generation systems are as follows:

- The MEA solvent in the CO₂ chemical absorption unit has a concentration of 30%wt [47–49].
- The suggested systems both operates under steady-state conditions [58,59].
- The utilized air contains 21% oxygen and 79% nitrogen [46,58].
- The changes in kinetic and potential energy are negligible [58,59].
- The C-100 and C-101 towers have IMTP packing [48,49].
- The drop in the pressure of heat exchangers and connections is negligible [60].

Schematic representations of the Aspen HYSYS modeling environment for the proposed System I (methane-based tri-generation) and System II (methane–geothermal multi-generation with MED) are provided in the *supplementary file*. Plus, the state properties of the main process streams in the proposed integrated combined cycle system are summarized in Table 2.

3. Methodology and materials

The study proposes an integrated framework for the evaluation and

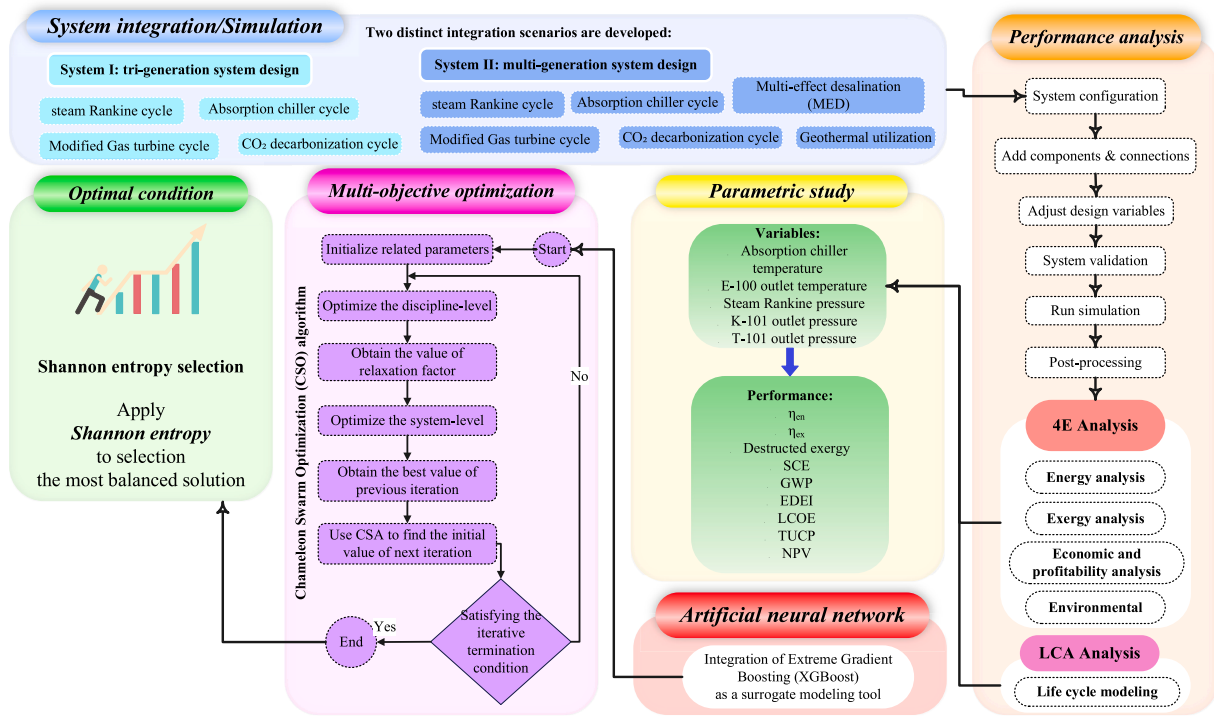


Fig. 4. The integrated framework for the evaluation and optimization of a simulated tri-generation system.

Table 3

The capital expenditure and operational expenditure calculation's assumption [82,84,85].

Parameter	Equation
Purchase cost of equipment (PCE)	$1 \times PCE_{2024}$
Installation cost of equipment	$0.39 \times PCE_{2024}$
Control and instrumentation cost	$0.26 \times PCE_{2024}$
Piping	$0.31 \times PCE_{2024}$
Direct costs (DC)	$1.96 \times PCE_{2024}$
Indirect costs (IDC)	$0.219 \times DC$
Fixed capital costs (FCC)	$DC + IDC$
Start-up costs	$0.05 \times FCC$
Capital expenditure	$FCC + \text{Start} - \text{Up Costs}$
Fixed operational expenditure	$0.03 \times \text{Capital Expenditure}$
Variable operational expenditure	(Methane cost + Water cost + Electricity cost + CO ₂ tax)
Methane cost factor (\$/GJ)	4
Water cost factor (\$/m ³)	1.5
Electricity cost factor (\$/kWh)	0.0775
CO ₂ tax	59.2
Operational expenditure	$\text{Fixed operational expenditure} + \text{Variable Operational expenditure}$

optimization of both simulated tri- and multi-generation systems that its process is depicted in Fig. 4. Under the evaluation part, a general performance investigation is conducted inclusive of energy and exergy performance analysis accompanied by comprehensive economic, and environmental analyses, and the investigations assisted by LCA. Furthermore, to acquire the optimum possible system performance, this study employs a machine learning-based multi-objective optimization process that enables the identification of efficient trade-offs among conflicting objectives and provides optimal design toward viable system implementations.

Table 4

The purchase cost function of equipment in carbon-neutral tri-generation system.

Component	Cost function	Base year	CEPCI _{Base year}
Pump [87]	$3540 \times [W_p]^f$	2011	586
CO ₂ capture unit [50,88]	$4.1811 \times 10^6 \times \dot{m}_{CO_2}^f \left(\frac{ton}{h} \right)$	2000	556.8
Heat exchanger [46]	$130 \times \left(\frac{A}{0.093} \right)^f$	2005	468.2
Compressor [87]	$\frac{71.1 \times \dot{m} \times P_{out}}{0.9 - \eta_{comp}} \ln \frac{P_{out}}{P_{in}}$	1995	368
Combustor [88]	$\frac{[1 + \exp((0.018T_5 - 26.4))] 46.08 \times \dot{m}_4}{0.995 - \frac{P_{in}}{P_{out}}}$	2001	394
Turbine [89,90]	$4405W^f$	2005	468.2
Gas turbine [91]	$\frac{266.3 \times \dot{m}_{10}}{0.92 - \eta_{GT}} \times \ln \left(\frac{P_{in}}{P_{out}} \right) \times (1 + \exp(0.036T_{10} - 54.4))$	1995	368

3.1. Energy and exergy performance modeling

Energy and exergy analyses are typically employed to quantitatively assess the thermodynamic performance of the proposed systems and to identify the potential for waste heat recovery and irreversibility reduction [61,62].

The energy performance of each system component is evaluated using the fundamental principles of mass and energy conservation. Eq. (8) represents the steady-state mass balance, ensuring continuity between inlet and outlet streams. Eq. (9) corresponds to the steady-flow energy balance, accounting for enthalpy transport by mass flows, heat transfer, and shaft work interactions. These equations form the basis for

```

1:  $P_p \leftarrow 0.1$  (the position update probability)
2:  $r_1, r_2, r_3, r_i$  are random numbers between 0 and 1
3:  $u$  and  $l$  are the upper and lower bounds of the search area
4:  $d \leftarrow$  dimension of the problem
5:  $y_{it}$  is the center of the current position of chameleon  $i$  at iteration  $t$ 
6:  $y_{rit}$  is the rotating centered coordinates of chameleon  $i$  at iteration  $t$ 
7: Randomly initialize the position of a swarm of  $n$  chameleons in the search space
8: Initialize the velocity of dropping chameleons' tongues
9: Evaluate the position of the chameleons
10: while ( $t < T$ ) do
11:   Define the parameter  $\mu$ 
12:   Define the inertia weight  $\omega$ 
13:   Define the acceleration rate  $a$ 
14:   for  $i = 1$  to  $n$  do
15:     for  $j = 1$  to  $d$  do
16:       if  $ri \geq P_p$  then
17:          $y_{t+1}^{i,j} = y_t^{i,j} + p_1(p_t^{i,j} - G_t^j)r_1 + p_2(G_t^j - y_t^{i,j})r_2$ 
18:       else
19:          $y_{t+1}^{i,j} = y_t^{i,j} + \mu((u^j - l^j)r_3 + l_b^j)sgn(rand - 0.5)$ 
20:       end if
21:     end for
22:   end for
23:   for  $i = 1$  to  $n$  do
24:      $y_{t+1}^i = y_t^i + y_t^i$ 
25:   end for
26:   for  $i = 1$  to  $n$  do
27:     for  $j = 1$  to  $d$  do
28:        $v_{t+1}^{i,j} = \omega v_t^{i,j} + c_1(G_t^j - G y_t^{i,j})r_1 + c_2(P_t^{i,j} - y_t^{i,j})r_2$ 
29:        $y_{t+1}^{i,j} = y_t^{i,j} + ((v_t^{i,j})^2 - (v_{t-1}^{i,j})^2)/(2a)$ 
30:     end for
31:   end for
32: Adjust the chameleons' positions according to  $u$  and  $l$ 
33: Evaluate the new positions of the chameleons
34: Update the position of the chameleons
35:  $t = t + 1$ 
36: end while

```

Fig. 5. The step-by-step algorithm of MOCOSO.

calculating component-level energy exchanges within the applied units [63,64].

$$\sum \dot{m}_{in} - \sum \dot{m}_{out} = 0 \quad (8)$$

$$\sum \dot{m}_{in} h_{in} + \dot{Q} - \sum \dot{m}_{out} h_{out} - \dot{W} = 0 \quad (9)$$

The terms h_{in} and h_{out} refer to the enthalpy of the specific stream, while $\dot{m}_{in}$ and $\dot{m}_{out}$ indicate its mass flow rates. The heat transfer rate $\dot{Q}$ and power rate $\dot{W}$ capture thermal and mechanical energy interactions, respectively. Using these balances, the useful energy outputs of each subsystem are determined and subsequently used to compute energy efficiencies.

To complement the energy analysis, an exergy-based framework is adopted to evaluate the quality of energy flows and quantify irreversibilities within the system. The total exergy rate of a stream (in the absence of kinetic and potential exergy) is decomposed into physical and chemical components, as expressed in Eq. (10) [65–67].

$$\dot{Ex}_{total} = \dot{Ex}_{ph} + \dot{Ex}_{ch} \quad (10)$$

Physical exergy ($\dot{Ex}_{ph}$) in Eq. (11) accounts for deviations of

temperature and pressure from the environmental dead state (T_0, P_0), while chemical exergy ($\dot{Ex}_{ch}$) in Eq. (12) reflects the departure of chemical composition from environmental equilibrium [65,68].

$$\dot{Ex}_{ph} = \dot{m}[(s_0 - s) \times (-h_0 + h) - T_0] \quad (11)$$

$$\dot{Ex}_{ch} = \dot{m} \left[\sum x_i e_{ch,i} - RT_0 \sum x_i \ln x_i \right] \quad (12)$$

Here, x_i indicates the fraction of mole, while $e_{ch,i}$ is the chemical exergy at standard condition.

The component-level exergy destruction rate, defined in Eq. (13), represents the irreversible losses caused by entropy generation within each unit. Based on this formulation, the rate of destructed exergy is introduced to identify the relative contribution of each component to total system irreversibility (Eq. (14)). Furthermore, the exergy efficiency in Eq. (15) quantifies how effectively the supplied exergy is converted into useful products (i.e. exergy efficiency for i -th component), providing a more rigorous performance metric than energy efficiency alone [69,70].

$$\dot{Ex}_{D,i} = \dot{Ex}_{F,i} - \dot{Ex}_{P,i} \quad (13)$$

Table 5

The outcome related to exergy-based parameters for carbon-neutral tri-generation system.

Component	$\dot{E}x_F$	$\dot{E}x_P$	$\dot{E}x_D$	ε_i	γ_i
K-100	721	675	46	0.936	0.01
K-101	661	610	51	0.922	0.011
K-102	742	703	39	0.947	0.0085
T-100	7335	7094	241	0.967	0.053
E-102	313	207	106	0.661	0.023
Reactor	12,599	9839	2760	0.781	0.6
E-100	138	87	51	0.63	0.011
P-100	13	10	3	0.769	0
E-103	1687	1384	303	0.82	0.066
E-104	675	596	79	0.882	0.017
T-101	808	747	61	0.924	0.013
E-101	171	140	31	0.82	0.0068
V-100	159	159	0	1	0
V-101	55	55	0	1	0
E-108	138	97	41	0.7	0.0089
VLV-101	20	14	6	0.7	0.0013
E-109	42	34	8	0.81	0.0017
VLV-102	38	29	9	0.763	0.0017
E-110	37	26	11	0.71	0.0024
E-111	35	24	11	0.69	0.0024
VLV-100	19	17	2	0.89	0.0004
P-102	4	3	1	0.75	0
E-105	165	114	51	0.69	0.011
C-100	65,865	65,699	166	0.997	0.036
P-101	7	6	1	0.857	0
E-106	314	255	59	0.812	0.013
E-107	110	89	21	0.81	0.0046
C-101	65,750	65,321	429	0.993	0.093

$$\gamma_i = \frac{\dot{E}x_{D,i}}{\sum \dot{E}x_{D,i}} \quad (14)$$

$$\varepsilon_i = 1 - \frac{\dot{E}x_{D,i}}{\dot{E}x_{F,i}} \quad (15)$$

Here, $\dot{E}x_{F,i}$ and $\dot{E}x_{P,i}$ refer the input and output exergy from fuel and products. The mass-energy and mass-exergy equations for system's components are provided in *supplementary file*.

Additionally, in the suggested tri-generation system, the main energy source is natural gas (methane), which the input energy and exergy from this source are determined as below:

$$\vartheta_f = \dot{m}_f \times LHV_f \quad (16)$$

$$\dot{E}x_f = \dot{E}x_{ph,f} + \dot{E}x_{ch,f} \quad (17)$$

Here, the calorific value of the fuel (LHV_f) is considered equivalent to 50,030 kJ/kg.

For the modified gas turbine cycle (MGTC), the energy efficiency is defined in Eq. (18) as the ratio of net useful work output and recovered thermal energy to the fuel energy input.

$$\psi_{MGTC} = \frac{\dot{W}_{T100} - \sum \dot{W}_K + \sum \dot{Q}_{recuperator}}{\vartheta_f} \quad (18)$$

where:

$$\sum \dot{Q}_{recuperator} = \dot{Q}_{E100} + \dot{Q}_{E101} \quad (19)$$

The absorption chiller (AC) coefficient of performance in Eq. (20) relates the cooling effect to the driving heat and pumping power,

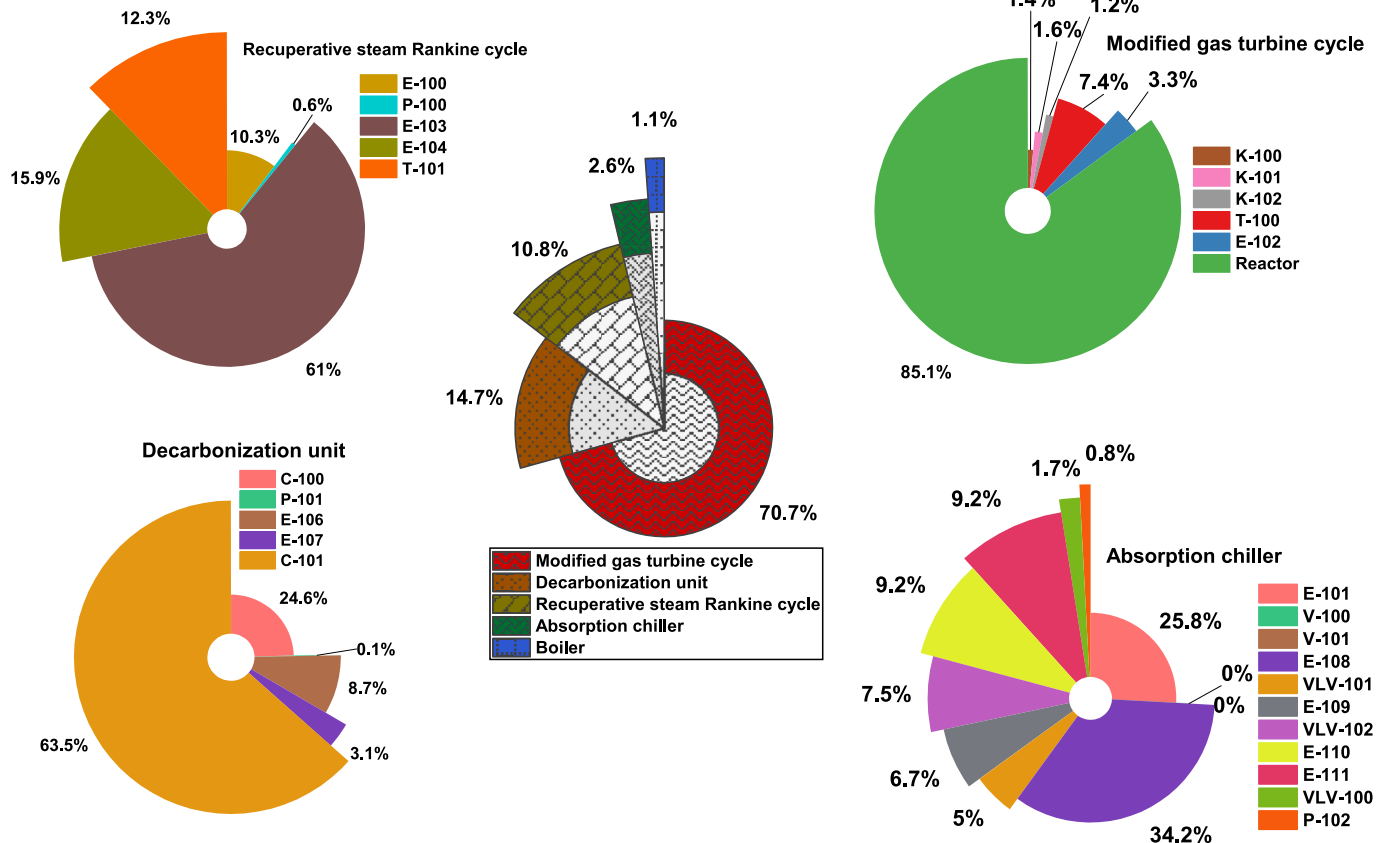


Fig. 6. The contribution of units and components in the destruction of tri-generation system' exergy.

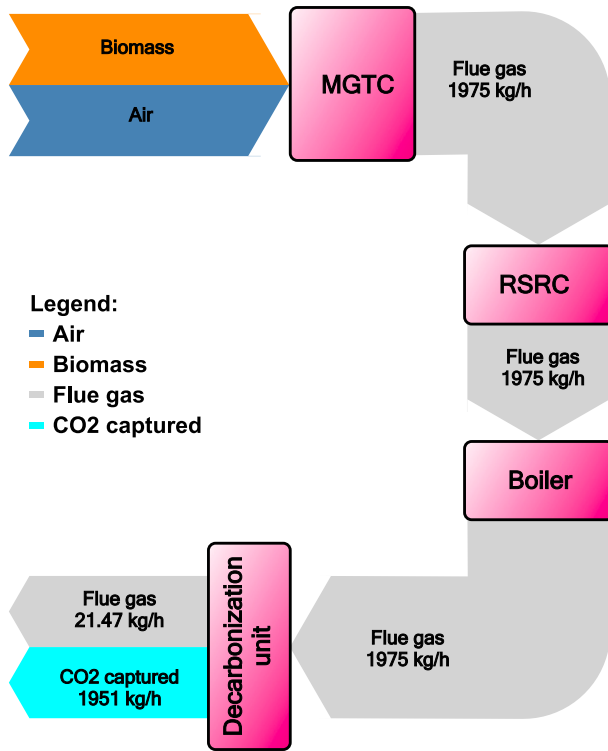


Fig. 7. The CO₂ emission mass balance within suggested carbon-neutral tri-generation system.

Table 6

The outcome related to global warming potential-based parameters for carbon-neutral tri-generation system.

Parameter	Value
GWP direct (kg/h)	23.7
GWP indirect (kg/h)	3020.4
Cooling (kW)	4922.0
Cooling water pumping (kg /h)	3020.4
GWP MEA	3.10
CO ₂ Capture (kg/h)	1951.5
GWP total (kg/h)	1095.74
Energy produced (kW)	6307.5
GWP per kWh (kg/kWh)	0.173

Table 7

The outcome related to capital and operational expenditures for carbon-neutral tri-generation system.

Parameter	Value (M\$)
Purchase cost of equipment	27.67
Installation cost of equipment	10.79
Control and instrumentation cost	7.19
Piping	8.58
Direct costs	54.23
Indirect costs	11.88
Fixed capital costs	66.11
Start-up costs	3.31
Capital expenditure	69.41
Fixed operational expenditure	2.08
Variable operational expenditure	2.05
Methane cost	1.23
Water cost	0.81
Electricity cost	0.00
CO ₂ tax	0.0099
Operational expenditure	4.14

$$\psi_{AC} = \frac{\dot{Q}_{evap}}{\dot{Q}_{E101} + \dot{W}_{P102}} \quad (20)$$

where:

$$\dot{Q}_{evap} = \dot{m}_{47}(h_{47} - h_{46}) \quad (21)$$

while the recuperative steam Rankine cycle (RSRC) efficiency in Eq. (22) measures the effectiveness of waste heat conversion into electricity.

$$\psi_{RSRC} = \frac{\dot{W}_{T101} - \dot{W}_{P100}}{\dot{Q}_{SG}} \quad (22)$$

where:

$$\dot{Q}_{SG} = \dot{m}_{12}(h_{12} - h_{13}) \quad (23)$$

The boiler heat production rate and CO₂ capture performance indicators are similarly defined based on energy and mass balances.

In the boiler, the heating production rate is defined based on Eq. (24):

$$\dot{Q}_{boiler} = \dot{m}_{13}(h_{13} - h_{20}) \quad (24)$$

In the CO₂ chemical absorption unit, the efficiency based on removed CO₂ (θ_{CO_2}) and the specific duty for reboiler (α_{reb}) are computed based on following equations [49,71]:

$$\theta_{CO_2} = 1 - \frac{\dot{m}_{CO_2,out}}{\dot{m}_{CO_2,in}} \quad (25)$$

$$\alpha_{reb} (MJ/kg) = \frac{\dot{Q}_{reboiler}}{\dot{m}_{CO_2}} \quad (26)$$

To evaluate the overall performance of the integrated tri-generation system, total energy and exergy efficiencies are defined in Eqs. (27) and (28), accounting for all useful outputs, including electricity, heating, and cooling.

$$\eta_{en} = \frac{\dot{W}_{net} + \dot{Q}_{boiler} + \dot{Q}_{evap}}{\dot{\theta}_f} \quad (27)$$

$$\eta_{ex} = \frac{\dot{W}_{net} + \dot{E}x_{boiler} + \dot{E}x_{evap}}{\dot{E}x_f} \quad (28)$$

where:

$$\dot{W}_{net} = - \sum \dot{W}_p - \sum \dot{W}_K + \sum \dot{W}_T \quad (29)$$

$$\dot{E}x_{boiler} = \dot{Q}_{boiler} \times \left(1 - \frac{T_0}{T_{22}} \right) \quad (30)$$

$$\dot{E}x_{evap} = \dot{Q}_{evap} \times \left(\frac{T_0}{T_{49}} - 1 \right) \quad (31)$$

Additionally, the Primary Energy Saving (PES) index in Eq. (32) is introduced to quantify the fuel savings achieved by the integrated configuration relative to conventional separate production systems [46,72]:

$$Primary\ Energy\ Saving = 1 - \frac{Energy\ consumption\ in\ current\ system\ (\dot{\theta}_f)}{Energy\ consumption\ in\ separate\ system\ (\dot{\theta}_{SP})} \quad (32)$$

where:

$$\dot{\theta}_{SP} = \frac{\dot{W}_{net}}{\psi_{elect}^{SP}} + \frac{\dot{Q}_{boiler}}{\psi_{th}^{SP}} + \frac{\dot{Q}_{evap}}{\psi_{elect}^{SP} \times COP_{SP}} \quad (33)$$

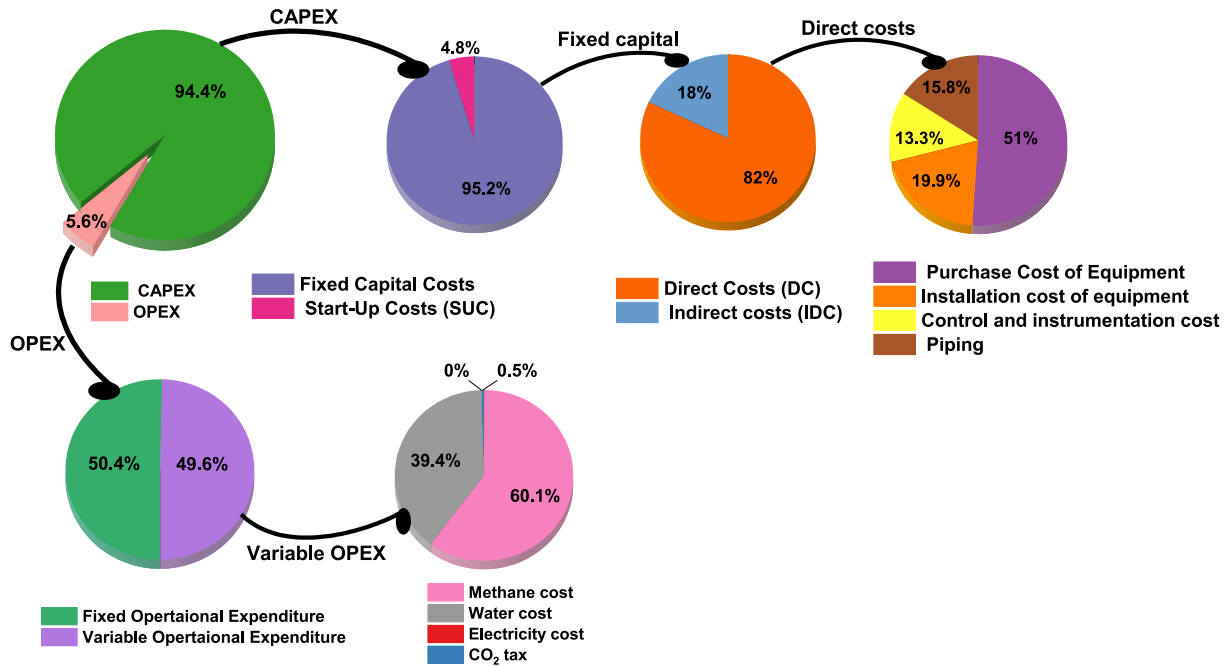


Fig. 8. The contribution of different costs in the capital and operational expenditures of tri-generation system.

Table 8

The outcome related to purchase cost of equipment for carbon-neutral tri-generation system.

Equipment	Base year's equipment cost (M\$)	2024's equipment cost (M\$)	2024's equipment cost rate (\$/h)
E-103	0.265	0.454	9.07
K-102	1.489	3.240	64.81
E-104	0.092	0.773	15.46
T-101	0.452	0.074	1.48
E-105	0.043	4.768	95.39
K-100	2.193	0.026	0.52
E-109	0.015	0.056	1.11
E-111	0.033	0.135	2.69
P-100	0.096	0.067	1.35
E-101	0.039	0.225	4.50
Reactor	0.111	0.023	0.45
E-108	0.013	2.978	59.58
K-101	1.370	4.753	95.09
T-100	2.186	0.123	2.46
E-100	0.072	0.025	0.51
E-110	0.015	0.093	1.85
E-102	0.054	0.028	0.55
P-102	0.020	0.157	3.14
CO ₂ capture	6.733	9.678	193.60

3.2. Environmental and life cycle modeling

Environmental analysis is performed to quantify the ecological impacts of the proposed tri-generation system and to evaluate its environmental sustainability in comparison with conventional energy production pathways. The assessment focuses on direct carbon emissions during operation, exergo-environmental indicators that link thermodynamic irreversibility with environmental impact, and life cycle-based global warming potential.

The Specific Carbon Emission (SCE), presented in Eq. (34), is used as a primary environmental performance indicator. This parameter represents the amount of carbon dioxide emitted per unit of net electrical power generated and allows a direct comparison with other power and tri-generation systems reported in the literature [73]. The total CO₂ emission rate includes combustion-related emissions from fuel

utilization, while emissions associated with upstream processes are considered in the LCA.

$$SCE \text{ (kg/kWh)} = \frac{\dot{m}_{CO_2}^{total}}{\dot{W}_{net}} \quad (34)$$

On the other side, in order to account for the combined thermodynamic and environmental performance, an exergo-environmental framework is adopted. The Environmental Damage Effectiveness Index (EDEI) in Eq. (35) relates the total exergy destruction to the useful exergy output of the system, thereby linking irreversibility with environmental degradation. This index provides insight into how efficiently the system converts resource exergy into useful products while minimizing environmental damage [74].

$$\text{Environmental Damage Effectiveness Index} = \frac{\dot{Ex}_{D,total}}{\eta_{exergy} \dot{Ex}_{F,total}} \quad (35)$$

Based on this formulation, the Exergo-environmental Impact Improvement index in Eq. (36) is introduced as an inverse indicator, where higher values correspond to lower environmental damage per unit of useful output [74]. In addition, the Exergetic Stability Factor in Eq. (37) evaluates the robustness of the system from an exergo-environmental perspective by accounting for the relative magnitude of destroyed, produced, and transferred exergy [74].

$$\text{Exergo-environmental Impact Improvement} = \frac{1}{\text{Environmental Damage Effectiveness Index}} \quad (36)$$

$$\text{Exergetic Stability Factor} = \frac{\dot{Ex}_{D,total}}{\dot{Ex}_{D,total} + \dot{Ex}_{P,total} + 1} \quad (37)$$

For a broader sustainability perspective, an LCA-based Global Warming Potential (GWP) assessment is conducted using Eq. (38) [75–77]. In this study, the LCA is defined as a gate-to-gate assessment, focusing on the operational phase of the tri- and multi-generation systems. The formula considers both direct emissions from system operation and indirect emissions associated with auxiliary energy consumption, while also explicitly accounting for the amount of CO₂ captured in the chemical absorption unit. Emissions from equipment

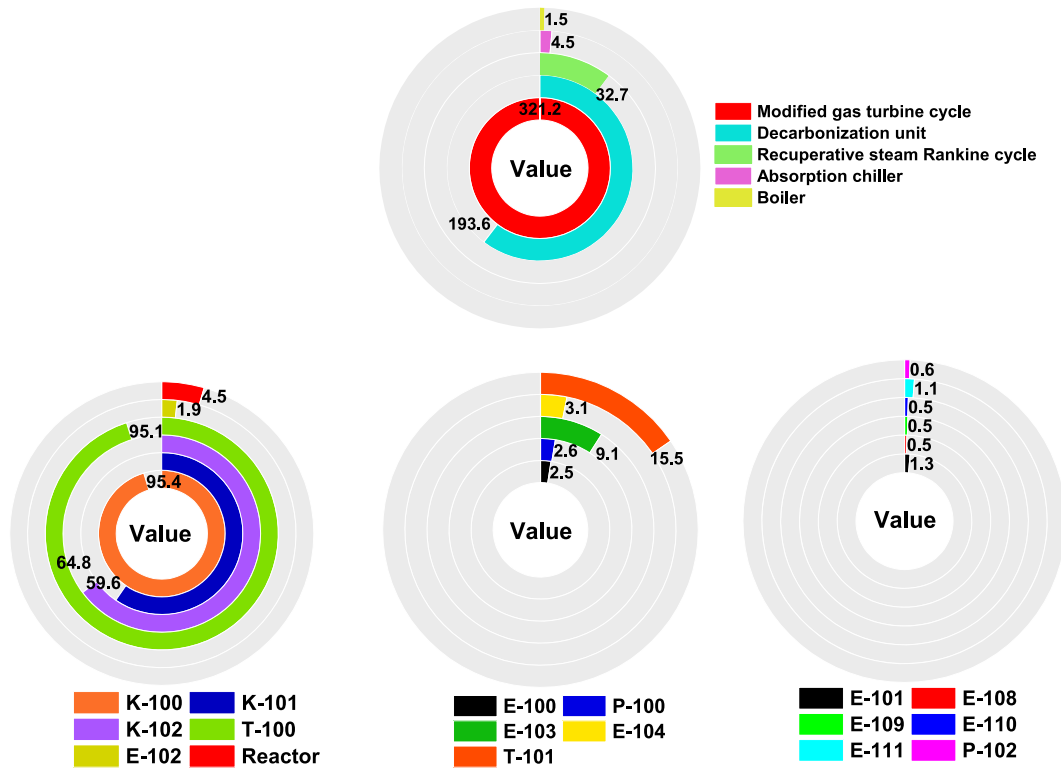


Fig. 9. The contribution of units and components in 2024's equipment cost rate of tri-generation system.

manufacturing, end-of-life recycling, MEA production/disposal, and refrigerant losses are excluded, as they are assumed identical across scenarios and thus do not affect the relative comparison. By integrating CO₂ capture effects, the proposed model provides a realistic estimate of the net climate impact of the operational system [75,76]:

$$\text{Total GWP (kg/h)} = \sum \text{GWP}_{\text{direct}} + \sum \text{GWP}_{\text{indirect}} - \text{captured CO}_2 \quad (38)$$

3.3. Economic and profitability modeling

Economic analysis is also carried out to evaluate the financial feasibility, cost competitiveness, and long-term profitability of the proposed tri-generation system. The modeling framework includes leveled cost indicators, capital and operational cost estimation, exergo-economic metrics, and standard investment evaluation criteria.

The Levelized Cost of Energy (LCOE), defined in Eq. (39), is employed as the principal economic performance indicator. LCOE represents the average cost of energy production over the system lifetime and enables a consistent comparison with alternative energy technologies [78].

$$\text{LCOE} = \frac{\text{Total annualized cost}}{N \times \sum \text{energy production}} \quad (39)$$

Here, N indicates the working hours for suggested tri-generation system, which is equal to 8000 h [79]. The total annualized cost in Eq. (40) combines capital recovery and operational expenditures, thereby capturing both investment and operating cost contributions [80]:

$$\text{Total annualized cost} = \text{Annualized Capital Expenditure} + \text{Operational Expenditure} \quad (40)$$

where [81,82]:

$$\text{Annualized Capital Expenditure} = \frac{i_r \times (1 + i_r)^j}{(1 + i_r)^j - 1} \times \text{Capital Expenditure} \quad (41)$$

$$\text{Operational Expenditure} = \text{Fixed Operational Expenditure} + \text{Variable Operational Expenditure} \quad (42)$$

Here, i_r refers to the rate of interest for suggested system, which is equal to 14% [79], while j indicates its operation years, which is equal to 20 years [83].

The Annualized Capital Expenditure in Eq. (41) is calculated using the capital recovery factor, which accounts for the time value of money through the interest rate and system lifetime. Operational expenditure in Eq. (42) is divided into fixed and variable components to reflect maintenance requirements and operating conditions, including fuel consumption, utilities, and environmental taxation. These assumptions are summarized in Table 3 to ensure transparency and reproducibility.

Purchase cost of equipment (PCE) is updated to the reference year (2024) using the Chemical Engineering Plant Cost Index (CEPCI), as shown in Eq. (43). This approach is widely adopted in techno-economic studies to normalize cost data from different base years and ensure consistency in economic evaluation [86]. The cost correlations and reference indices for major components are provided in Table 4.

$$\text{PCE}_{2024} = \text{PCE}_{\text{Base year}} \times \frac{\text{CEPCI}_{2024}}{\text{CEPCI}_{\text{Base year}}} \quad (43)$$

Here, the CEPCI_{2024} is equal to 800.5 [86].

Moreover, for integrating thermodynamic and economic perspectives, an exergo-economic analysis is conducted using the Total Unit Cost of Product (TUCP), defined in Eq. (44). This metric expresses the cost per unit of useful exergy output and reflects both capital investment and fuel consumption [92]:

$$\text{TUCP} (\$/\text{GJ}) = \frac{i_r \times (1 + i_r)^j}{(1 + i_r)^j - 1} \times \frac{(\varphi \times \sum \text{PCE}_{2024}) + \text{Fuel cost rate}}{\sum \text{exergy production} \times N} \quad (44)$$

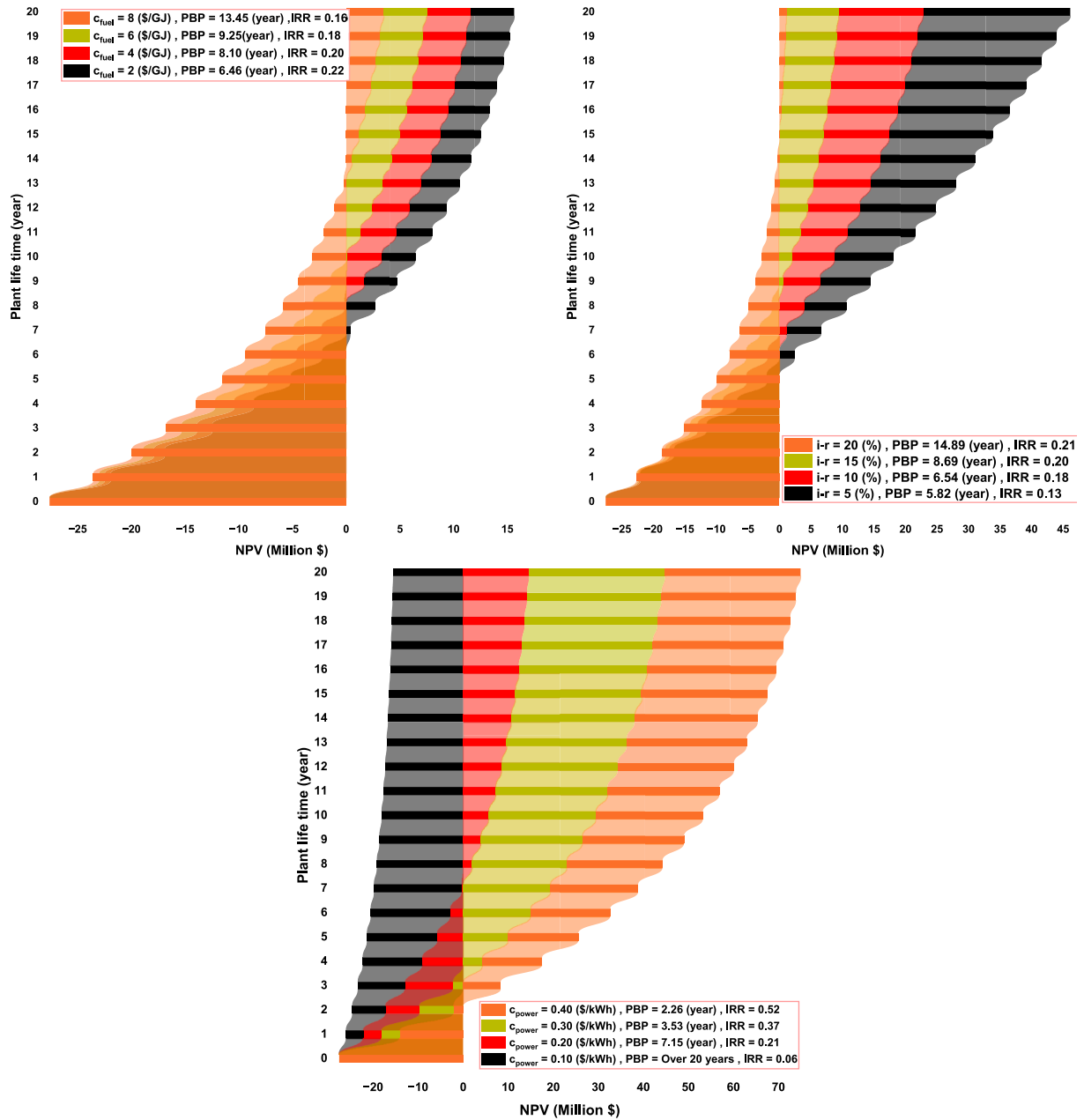


Fig. 10. The analysis of tri-generation system's profitability based on different economical parameters.

Here, φ refers to the maintenance factor for suggested tri-generation system, which is considered equal to 1.06 [92]. The fuel cost rate is also computed based on the lower heating value of methane and prevailing market prices, as expressed in Eq. (45) [79]:

$$\text{Fuel cost rate} = \text{Fuel cost factor} \times \vartheta_f \times N \quad (45)$$

In this study, the *fuel cost factor* for methane is equivalent to 4 \$/GJ [92].

Finally, profitability indicators, including Net Present Value (NPV) [92,93], Payback Period (PBP) [92], and Internal Rate of Return (IRR) [94], are employed to assess the investment attractiveness of the proposed system. These indicators consider annual revenues from electricity, heating, and cooling production, as well as operational expenditures, and are calculated using standard financial formulations (Eqs. 46–48). Together, these metrics provide a comprehensive evaluation of the economic viability and investment potential of the tri-generation system.

$$NPV = - \sum PCE_{2024} + (\text{Annual Income} - \text{Operational Expenditure}) \times \frac{i_r \times (1 + i_r)^j}{(1 + i_r)^j - 1} \quad (46)$$

$$PBP = \frac{\sum PCE_{2024}}{\text{Annual Income} - \text{Operational Expenditure}} \quad (47)$$

$$IRR = \frac{\text{Annual Income} - \text{Operational Expenditure}}{\sum PCE_{2024}} \left[1 - \frac{1}{(1 + IRR)^n} \right] \quad (48)$$

Here, *Annual Income* is computed based on cooling price of 0.08 \$/kWh [95], heating price of 0.018 \$/kWh [96] and electricity price of 0.19 \$/kWh [97].

3.4. Machine learning and multi-objective optimization modeling

The study applies a machine learning-aided multi-objective

Table 9

The outcome related to performance evaluation for carbon-neutral tri-generation system.

Parameter	Value
Thermodynamic outcomes	
Fuel energy inlet (kW)	10,010
Fuel exergy inlet (kW)	10,710
Geothermal energy inlet (kW)	4202
Geothermal exergy inlet (kW)	1037
Total generated power (kW)	5702
Total generated heating (kW)	465
Total generated heating modified (kW)	3404
Total generated cooling (kW)	141
Primary energy saving (%)	44.25
Tri-generation energy efficiency	63.03
CO ₂ removal efficiency (%)	98.78
Specific reboiler duty (MJ/kg)	4.14
Tri-generation exergy efficiency (%)	54.00
Modified gas turbine cycle efficiency (%)	62.91
Absorption chiller efficiency (%)	19.05
Recuperative steam Rankine efficiency (%)	23.78
Fresh water rate (kg/h)	4850.07
Environmental and life cycle outcomes	
Specific carbon emission (kg/kWh)	0.003766
Environmental damage effectiveness index (–)	0.8519
Exergo-environmental impact improvement (–)	1.174
Exergetic stability factor (–)	0.46.00
Total global warming potential (kg/h)	1095.74
Global warming potential (kg/kWh)	0.173
Economic and profitability outcomes	
Total annualized cost (M\$)	14.62
Purchase cost of equipment (M\$)	27.67
Purchase cost of equipment rate (\$/h)	553.53
Fuel cost rate (\$/h)	154.20
Total cost rate (\$/h)	707.73
Annualized capital expenditure (M\$)	10.48
Operational expenditure (M\$)	4.14
Levelized cost of energy (\$/kWh)	0.2897
Total unit cost of product (\$/GJ)	34
Net present value (M\$)	11.60
Payback period (year)	8.10
Internal return rate (%)	0.1987

optimization framework to determine the optimal operating conditions of the suggested carbon-neutral systems by considering performance priorities and given constraints [98]. The selected design parameters for optimization include the absorption chiller temperature (T_{AC} ranging 115–155 °C), E-100 outlet temperature (T_5 ranging 50–80 °C), steam Rankine cycle pressure (P_{RSRC} ranging 7000–9000 kPa), K-101 outlet pressure (P_6 in 1000–1800 kPa), and T-101 outlet pressure (P_{16} with 200–300 kPa).

The optimization methodology consists of two sequential phases. In the first phase, the thermodynamic behavior of the system simulated in Aspen HYSYS is approximated using an XGBoost regression model implemented in a Python environment [98–100]. A total dataset of 6221 samples was generated from Aspen HYSYS simulations and preprocessed prior to modeling. The dataset was randomly split into training (80%, 4976 samples) and testing (20%, 1245 samples) subsets to ensure unbiased performance evaluation. The predictive accuracy of the XGBoost

model was assessed using mean absolute error (MAE), root mean square error (RMSE), mean absolute percentage error (MAPE), and coefficient of determination (R^2), confirming the reliability of the surrogate model for subsequent optimization [101].

In the second phase, the trained machine learning model is integrated with multi-objective metaheuristic optimization algorithms to maximize exergy efficiency and minimize the total unit cost of the product. Four algorithms, including Multi-Objective Ant Colony Optimization (MOACO) [102], Multi-Objective Particular Swarm Optimization (MOPSO) [103], Multi-Objective Ant Lion Optimization (MOALO) [104] and Multi-Objective Chameleon Swarm Optimization (MOCSSO) [105], are evaluated and compared. The Python-based optimization algorithms directly communicate with the trained surrogate model to update decision variables, execute simulations, and retrieve objective function values. Convergence is ensured through two complementary mechanisms: (i) Aspen HYSYS's built-in convergence checker guarantees numerical stability of each simulation, and (ii) Python termination criteria halt the optimization when no significant improvement in objective functions is observed across successive generations. For all optimization algorithms, the maximum number of iterations was set to 500, and convergence was achieved by minimizing the mean squared error (MSE) between successive generations, with the optimization terminated when no further improvement in the objective functions was observed.

In addition, Shannon entropy decision-making method is applied, aiding in identifying the most balanced solution from the Pareto-optimal set. This method objectively assigns weights to each objective according to the amount of information they convey, thereby avoiding subjective or arbitrary weighting [106]. First, the normalized decision matrix (R_{ij}) is constructed using Eq. (49), where each objective value is normalized with respect to the sum of its corresponding objective across all Pareto solutions. Based on this matrix, the Shannon entropy of the j -th objective, SE_j , is calculated using Eq. (50). The entropy value reflects the degree of dispersion of each objective; lower entropy indicates greater variability and higher decision-making importance [107,108].

$$SE_j = -\frac{1}{\ln(n)} \sum_{i=1}^n R_{ij} \ln R_{ij} \quad (49)$$

Table 11

The XGBoost's performance evaluation outcomes in prediction of carbon-neutral tri-generation system's parameters.

	Target	RMSE	MAE	R^2	MAPE
Train	η_{ex}	0.0088	0.0068	0.9996	0.0127
	TUCP	0.0059	0.0046	0.9995	0.0134
	NPV	0.0110	0.0084	0.9996	0.0752
	SCE	0.0000	0.0000	0.3431	0.3955
	GWP	0.0008	0.0006	0.9990	0.3107
Test	η_{ex}	0.0131	0.0104	0.9991	0.0195
	TUCP	0.0088	0.0068	0.9990	0.0197
	NPV	0.0162	0.0125	0.9992	0.1121
	SCE	0.0000	0.0000	0.3413	0.3985
	GWP	0.0009	0.0007	0.9985	0.3789

Table 10

Comparison of energy, exergy, economic, and carbon performance of the proposed integrated systems versus literature-reported multi-generation systems.

Study	Outputs	Energy efficiency (%)	Exergy efficiency (%)	LCOE (\$/kWh)	SCE (kg/kWh)
[109]	Power, heating, cooling, freshwater, and hydrogen	26.95	33.76	0.472	0.2025
[110]	Power, heating, and cooling	23.04	26.55	–	–
[111]	Power, heating, cooling, and hydrogen	10.69	48.53	–	–
[73]	Power, heating, cooling, and freshwater	–	22.20	–	0.5180
This study; System I (Base condition)	Power, heating, and cooling	63.03	54.00	0.289	0.0037
This study; System II (Base condition)	Power, heating, cooling and freshwater	65.50	54.51	0.199	0.0037

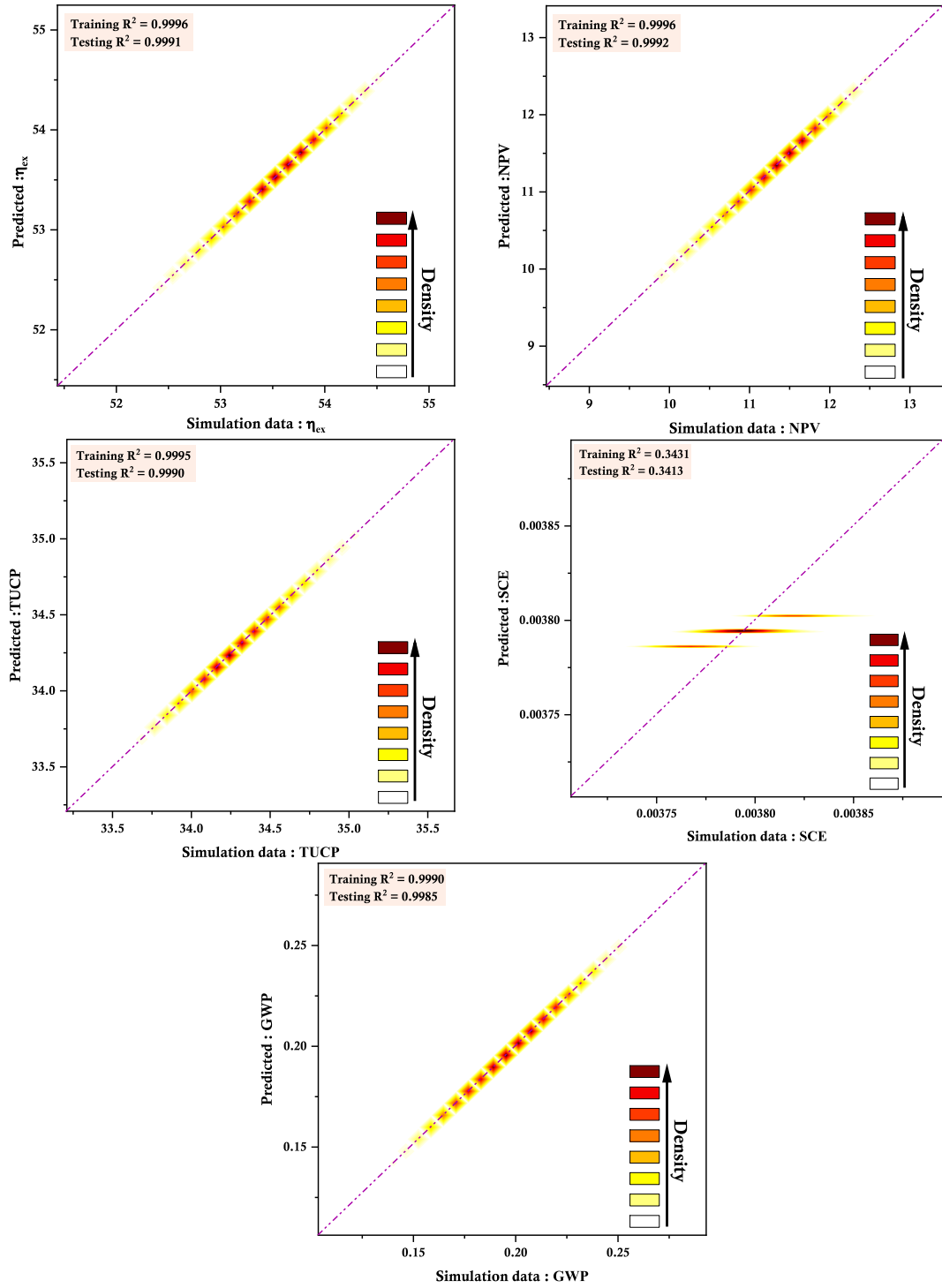


Fig. 11. The XGBoost's accuracy analysis based on distribution of predicted data around simulation data for critical parameters.

$$R_{ij} = \frac{F_{ij}}{\sum_{i=1}^n F_{ij}} \quad (50)$$

Next, the deviation degree (dd_j) is determined using Eq. (51), which quantifies the useful information provided by each objective. The normalized entropy-based weight (w_j) of each objective is then obtained using Eq. (52). Objectives exhibiting higher deviation degrees are assigned larger weights, reflecting their stronger influence on the decision-making process [107,108].

$$dd_j = 1 - SE_j \quad (51)$$

$$w_j = \frac{dd_j}{\sum_{j=1}^m dd_j} \quad (52)$$

Subsequently, an assessment parameter (x_i) is calculated for each solution using Eq. (53) by combining the normalized objective values with their corresponding weights. The solution with the maximum x_i is identified as the most balanced optimal design [107,108].

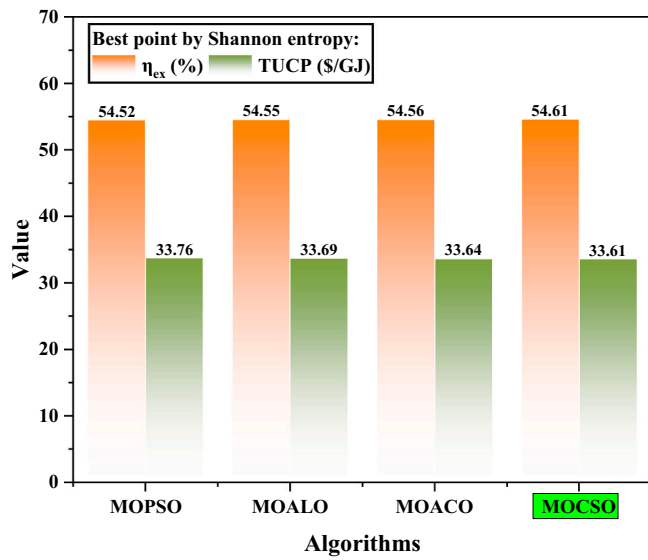


Fig. 12. The outcomes of bi-objective optimization process using four algorithms of MOPSO, MOALO, MOACO, and MOCOSO.

$$x_i = R_{ij} \cdot w_j \quad (53)$$

Finally, the deviation index defined in Eq. (54) is used to evaluate the distance of each Pareto solution from the ideal and anti-ideal solutions, ensuring that the selected design represents a rational compromise among all objectives [107,108].

$$d = \frac{\sqrt{\sum_{j=1}^n (F_j - F_j^{ideal})^2}}{\sqrt{\sum_{j=1}^n (F_j - F_j^{ideal})^2} + \sqrt{\sum_{j=1}^n (F_j - F_j^{nadir})^2}} \quad (54)$$

This entropy-based framework provides a transparent, data-driven, and robust mechanism for selecting the final optimal solution in multi-objective energy system optimization and has been widely applied in similar thermodynamic and sustainability-oriented studies [107,108].

Next, comparative analysis shows that the MOCOSO algorithm achieves the best trade-off between maximum exergy efficiency and minimum unit cost. Consequently, MOCOSO is selected for detailed optimization, and its step-by-step procedure is illustrated in Fig. 5.

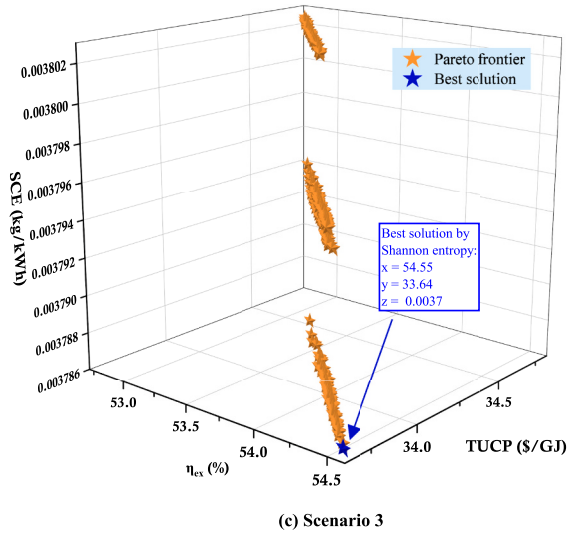
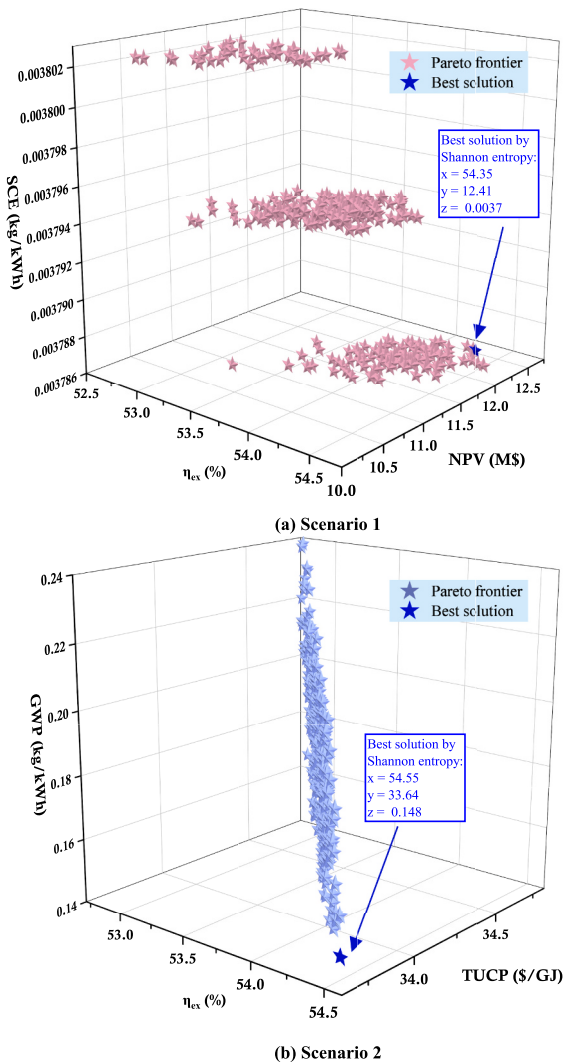


Fig. 13. The outcomes of tri-objective optimization process using MOCOSO algorithm.

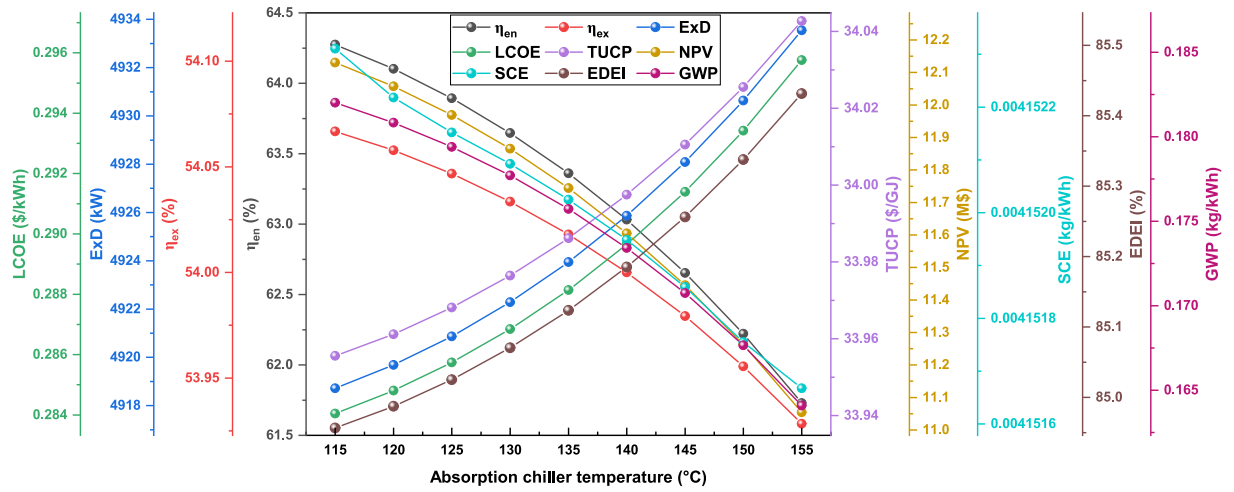


Fig. 14. The absorption chiller temperature's influences on η_{en} , η_{ex} , $\dot{E}x_D$, SCE, GWP, EDEI, LCOE, TUCP, and NPV.

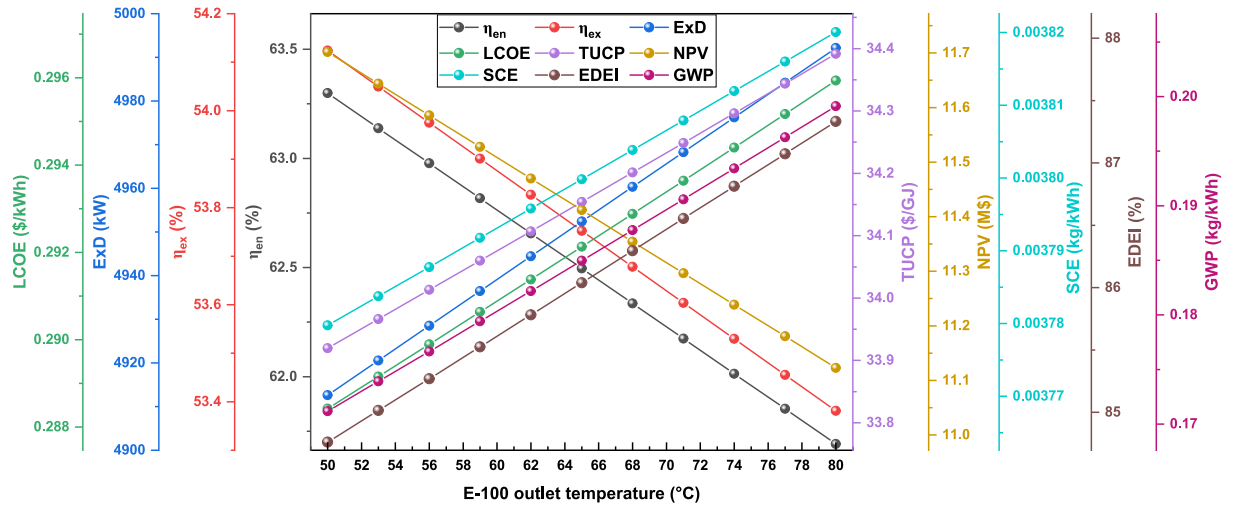


Fig. 15. The E-100 outlet temperature's influences on η_{en} , η_{ex} , $\dot{E}x_D$, SCE, GWP, EDEI, LCOE, TUCP, and NPV.

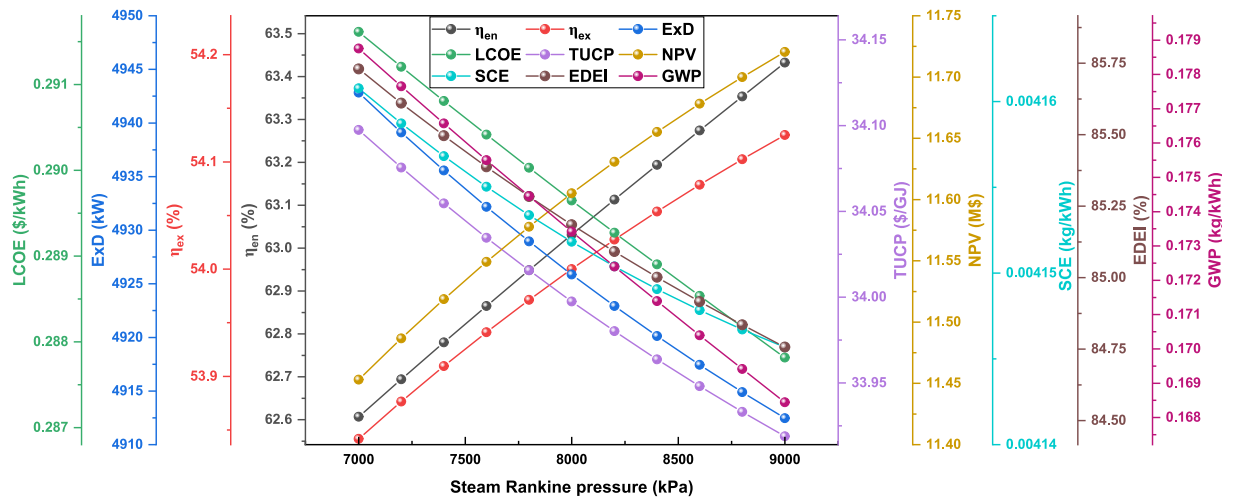


Fig. 16. The steam Rankine pressure's influences on η_{en} , η_{ex} , $\dot{E}x_D$, SCE, GWP, EDEI, LCOE, TUCP, and NPV.

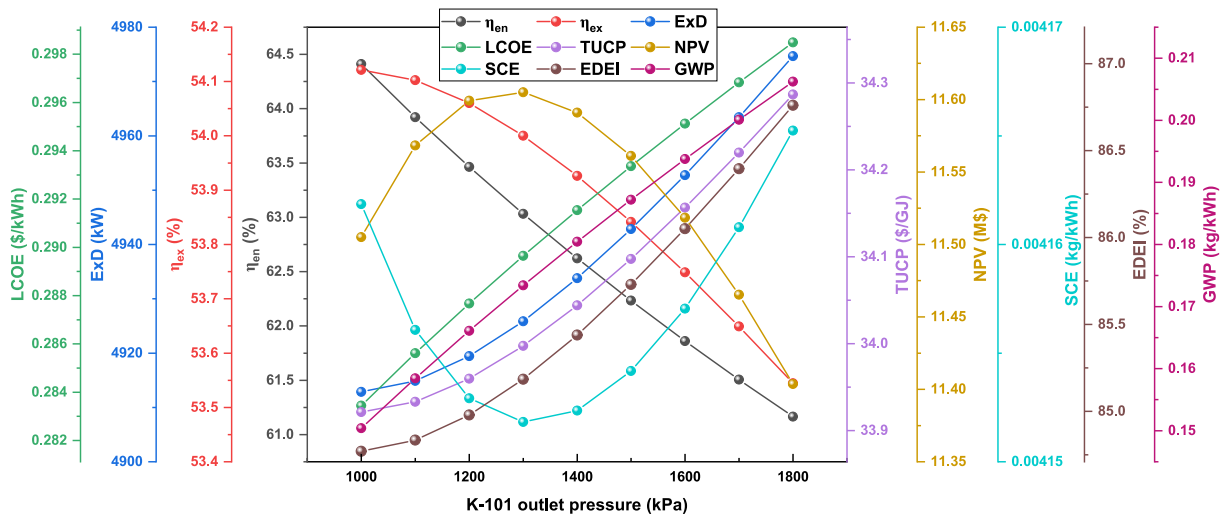


Fig. 17. The K-101 outlet pressure's influences on η_{en} , η_{ex} , $\dot{E}x_D$, SCE, GWP, EDEI, LCOE, TUCP, and NPV.

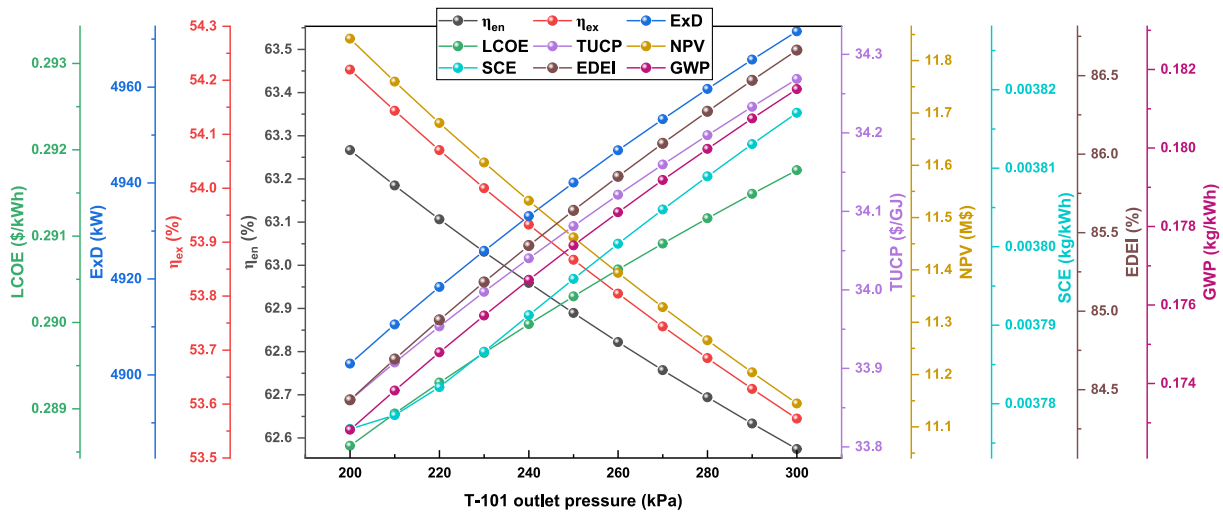


Fig. 18. The T-101 outlet pressure's influences on η_{en} , η_{ex} , $\dot{E}x_D$, SCE, GWP, EDEI, LCOE, TUCP and NPV.

4. Outcomes and discussion

4.1. System validation outcomes

In this research, the simulation procedure is verified in the *supplemental file* in order to assess the system simulation trustworthiness.

4.2. First scenario outcomes (System I)

4.2.1. Performance evaluation outcomes for tri-generation system

According to the main numerical results from the exergy analysis in Table 5, the system experiences a total of 4585 kW of exergy destruction due to irreversibility. As shown in Fig. 6, the modified gas turbine unit is the primary cause of the destruction, contributing 70.7% or 3243 kW of the total suggested tri-generation system. In this unit, the reactor is identified as the critical hotspot with an exergy destruction of 2760 kW due to the nature of combustion reactions, which explains the significant portion of this section. The second significant source for destruction of system's exergy is the decarbonization unit, accounting for 14.7% or 676 kW of the irreversibility in the system. Among the decarbonization components, the C-101 tower alone contributes 429 kW, reflecting the highest destruction share of 63.5%.

The mass balance of CO₂ emissions in the suggested carbon-neutral tri-generation system is shown in Fig. 7. As can be seen, the reactor produces about 1975 kg/h of CO₂ when methane fuel is burned, which stays constant as the flue gas moves through the water boiler and steam Rankine. Finally, directing the flue gas to the decarbonization unit enables the MEA solvent to capture 98.78% of the CO₂, resulting in a mass-based capture efficiency of 98.78%. As a result, only around 21.47 kg/h of CO₂ is eventually released into the atmosphere, with the 1951 kg/h of CO₂ being efficiently absorbed inside the system.

According to the results of global warming potential in Table 6, the system's indirect GWP, which is mostly related to auxiliary processes like cooling water pumping, reaches 3020.4 kg/h, while its direct GWP is comparatively low at 23.7 kg/h. However, by integrating a decarbonization unit, 1951.5 kg/h of CO₂ is removed, resulting in a significant reduction in total GWP to 1095.74 kg/h. Crucially, the suggested tri-generation system's specific GWP per unit of energy generated is only 0.173 kg/kWh, showing that it is highly effective at reducing greenhouse gas emissions when compared to traditional fossil fuel-based system.

Table 7 demonstrates the breakdown of capital and operating expenses for proposed carbon-neutral tri-generation system. Based on the calculation, the total investment is estimated at 69.41 M\$ for capital

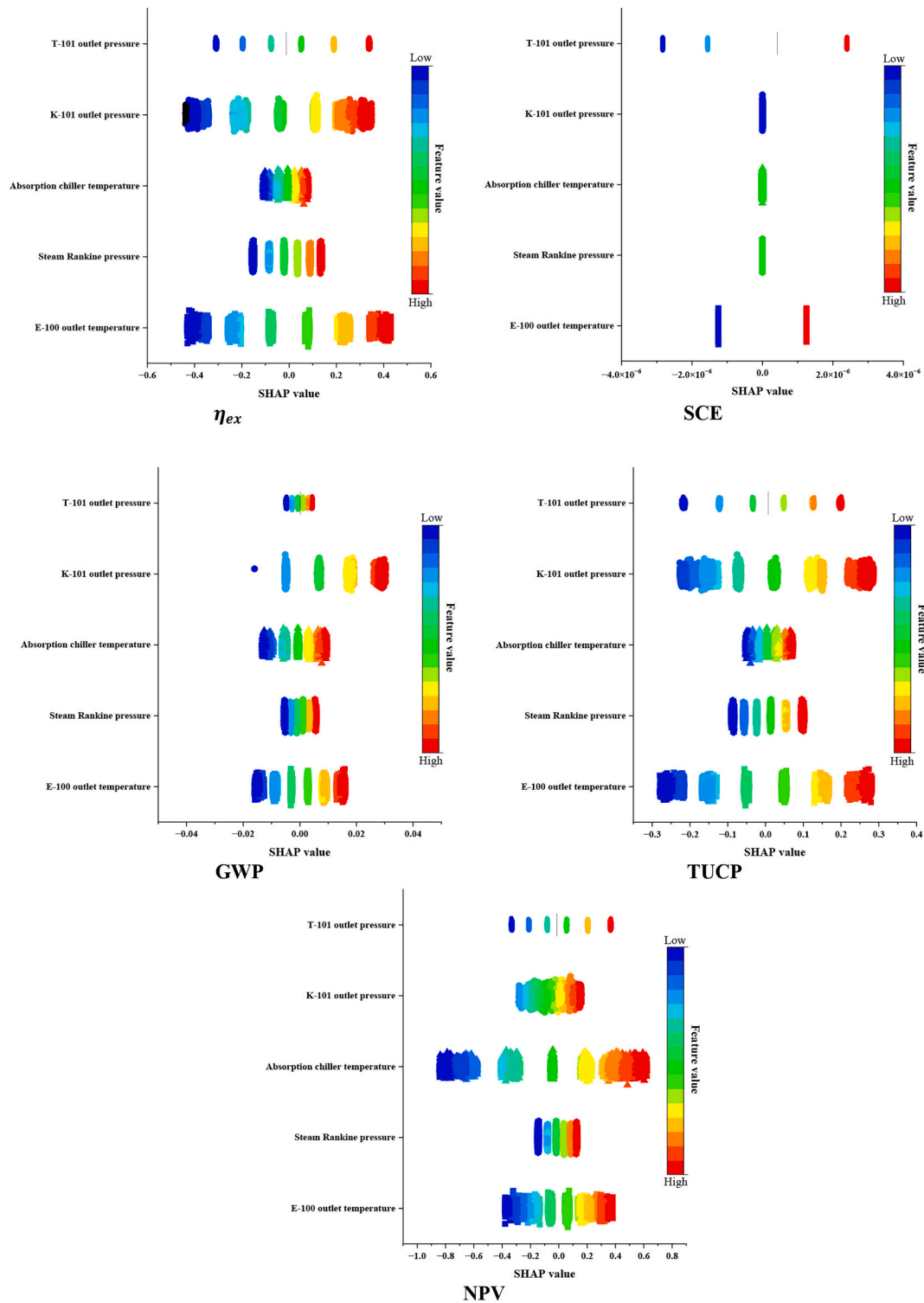


Fig. 19. The SHAP sensitivity analysis of η_{ex} , SCE, GWP, TUCP and NPV on design parameters.

costs and 4.14 M\$ for operational expenses, and Fig. 8 depicts the contribution of different costs in these expenditures. From this figure it can be seen that, only 4.8% of capital expenditures are devoted to start-up costs, with the vast majority around 95.2% going toward fixed capital requirements. Upon closer examination, direct costs make up 82% of fixed capital, while indirect costs make up the remaining 18%. In term of operational expenses, 49.6% of this expense come from variable costs, which are heavily reliant on changes in utility consumption prices, and 50.4% come from fixed costs.

Table 8 summarizes the purchase cost for equipment's tri-generation system, and Fig. 9 shows the relative contributions of different units and components to the equipment cost rate in 2024 year. Based on the figure, the cost rate of gas turbine unit is the system's largest contributor, making up 321.2 \$/h of the overall cost rate. Within this unit, the T-100 turbine contributes 95.1 \$/h, while the compressors K-100, K-101, and K-102 contribute 95.4 \$/h, 59.6 \$/h, and 64.8 \$/h of gas turbine unit's cost rate, that together account for a sizeable amount of the equipment cost rate.

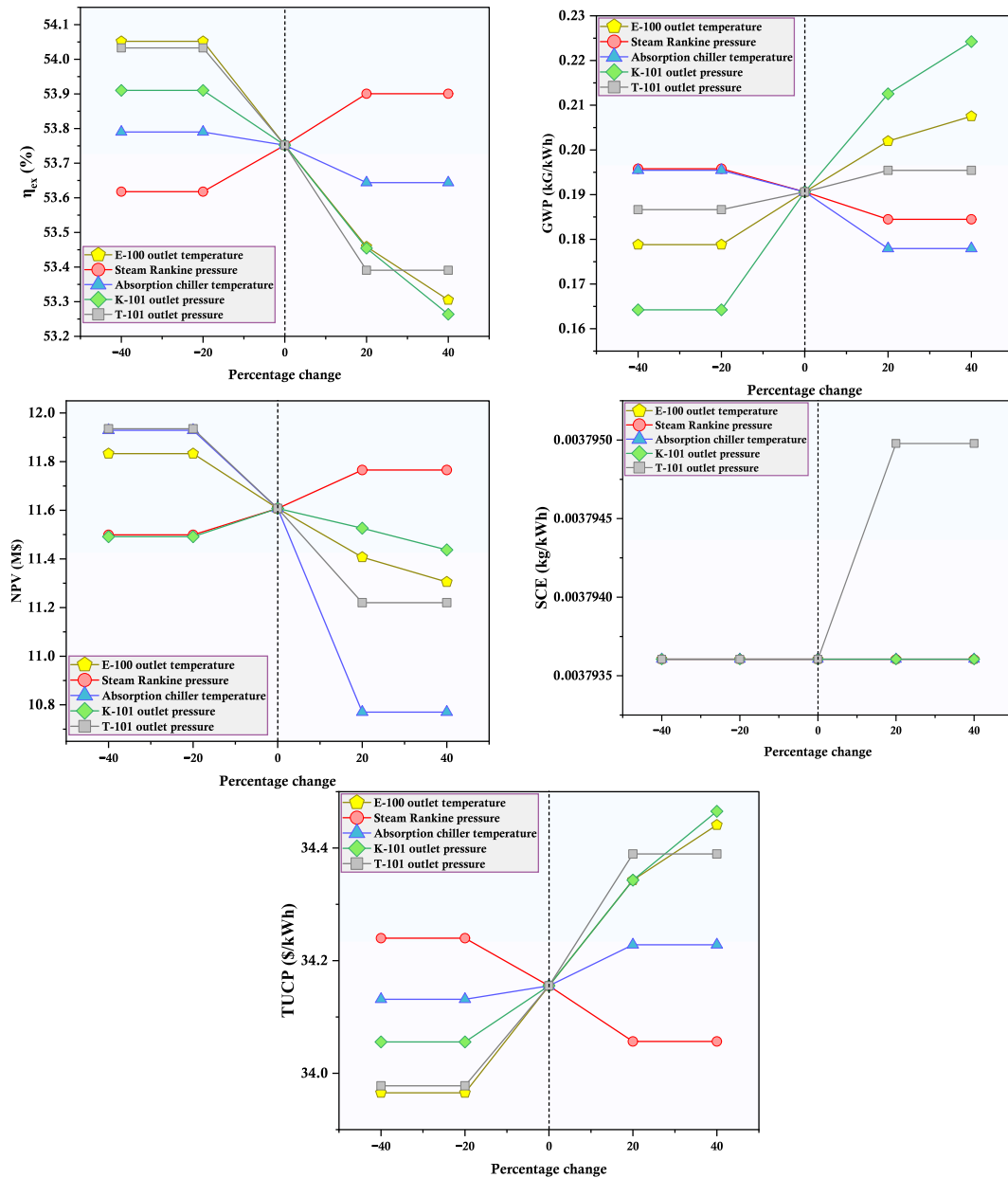


Fig. 20. The Morris sensitivity analysis of η_{ex} , SCE, GWP, TUCP, and NPV on design parameters.

The tri-generation system's profitability evaluation under various economic conditions is shown in Fig. 10. According to the analysis, the system's net present value drops to almost 3.43 M\$ by the 20th year in the suggested configuration when the fuel price rises to 8 \$/GJ and the interest rate rises to 16%. This decline results from the detrimental effects of increased fuel prices and higher financing costs, which increase operating costs and lower yearly revenue. On the other hand, the system reacts favorably to increases in the cost of electricity so that the value of net present increases to almost 75 M\$ when the electricity tariff is raised from 0.10 \$/kWh to 0.40 \$/kWh, driven by higher annual revenues from power generation. This increased profitability highlights the system's economic feasibility in advantageous market conditions by resulting in a shorter payback period and a more alluring rate of return.

Based on the performance evaluation outcomes in Table 9, the carbon-neutral tri-generation system achieves efficiencies of 63.03% and 54.00% for generated energy and exergy, by producing 5702 kW of power, 465 kW of heating, and 141 kW of cooling. The decarbonization unit provides a very high CO₂ removal efficiency of 98.78%, reducing

emissions to just 21.47 kg/h which results lower global warming potential to 0.173 kg/kWh for generated energy. Economically, the system shows strong feasibility, with a leveled cost of energy of 0.2897 \$/kWh, and a net present value of 11.6 M\$ and a payback period of 8.1 years.

Furthermore, as shown in Table 10, the proposed methane-based System I and methane-geothermal System II achieve higher energy and exergy efficiencies compared to previous studies, while substantially lowering specific carbon emissions. The LCOE values of the proposed systems are competitive, highlighting their thermo-economic viability alongside improved environmental performance.

4.2.2. XGBoost modeling outcomes

Based on the XGBoost's performance evaluation outcomes in Table 11, the developed model demonstrates outstanding accuracy across the majority of evaluation targets. This model in both training and test datasets, for all target parameters show extremely low error values based on RMSE, MAE, MAPE metrics and invariably high

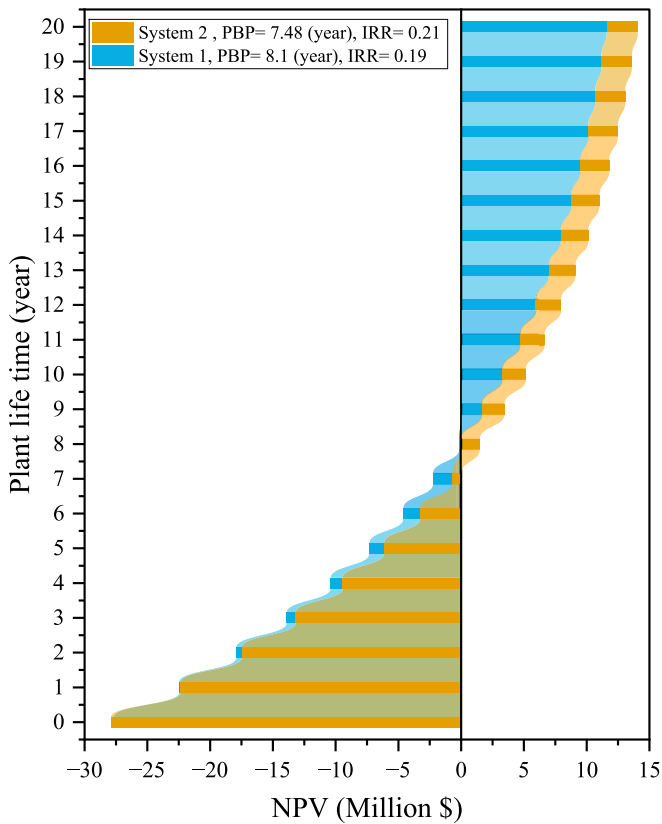


Fig. 21. NPV comparison over 20 years for System I (methane tri-generation) and System II (methane-geothermal multi-generation).

Table 12

Comparison of thermo-enviro-economic performance indicators for System I vs. System II.

Parameters	System I	System II
Primary energy saving (%)	44.25	52.99
Tri-generation energy efficiency	63.03	65.50
Tri-generation exergy efficiency	54.00	54.51
Purchase cost of equipment (M\$)	27.7	27.9
Net present value (M\$)	11.60	14.07
Payback period (year)	8.1	7.48
Internal return rate	0.1987	0.2106
Levelized cost of energy (\$/kWh)	0.2897	0.1998
Total unit cost of product (\$/GJ)	34	32.35
Global warming potential (kg/kWh)	0.173	0.0179

accuracy based on $R^2 > 0.998$, validating eminent generalization ability. Furthermore, in Fig. 11 the comparison between the predicted values and the simulation data for these parameters reveals a close and well-balanced distribution around the reference line, indicating that the model successfully captures the inherent trends and variability of the system. The XGBoost model with the predicted points clustering tightly around the 1:1 line demonstrates minimal deviation and confirms the strong agreement between predictions and simulations. Overall, the results confirm that the XGBoost approach provides highly accurate and stable predictions, which make it reliable for application in optimization process.

4.2.3. Multi-objective optimization outcomes

Fig. 12 shows the results of the bi-objective optimization process for the suggested carbon-neutral tri-generation system, which used four metaheuristic algorithms including MOPSO, MOALO, MOACO, and MOCSO. The goal of the optimization task was to minimize the total unit

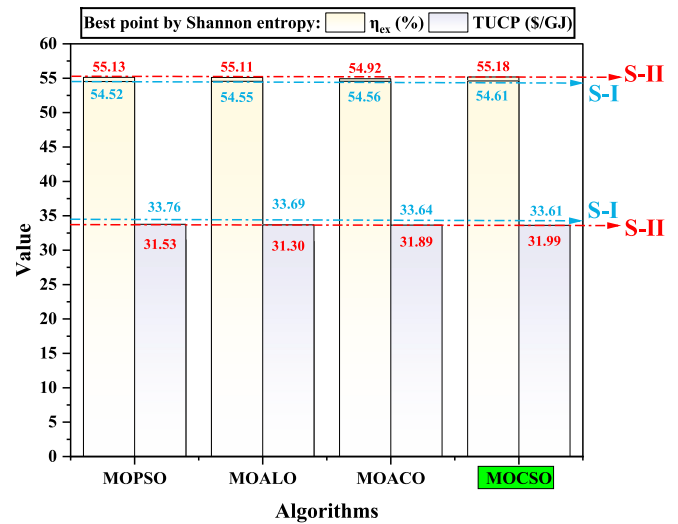


Fig. 22. The comparative outcomes of two-objective optimization via four MOPSO, MOALO, MOACO, and MOCSO algorithms in terms of System I vs. System II.

cost of product, while simultaneously increasing the system's exergy efficiency. According to a comparative analysis, despite that the majority of the algorithms can achieve satisfactory trade-offs between technical and economic goals, the MOCSO produces strong performance across the assessed metrics with the most optimist solution. Based on this figure, the MOCSO algorithm with the help of Shannon entropy achieves the most optimal solution with the highest η_{ex} of 54.61% and the lowest TUCP value of 33.61 \$/GJ.

Fig. 13 indicates the outcomes of tri-objective optimization process using MOCSO algorithm, which underscore the effect of shifting priorities across scenarios. In Scenario 1, where net present value is included as a distinguished objective, the system achieves a balanced outcome with moderate η_{ex} of 54.35% and strong economic profitability with NPV of 12.41 M\$, while sustaining low emissions with SCE of 0.003 kg/kWh. By contrast, Scenario 2 removes direct profitability and sustainability from the optimization objectives, focusing instead on reducing TUCP and GWP. This shift improves efficiency with η_{ex} of 54.55% and lowers TUCP to 33.64 \$/GJ, while also addressing climate impact with a GWP of 0.14 kg/kWh. By combining TUCP reduction and SCE minimization, Scenario 3 builds on the benefits of Scenario 2, resulting in the same η_{ex} of 54.55% and TUCP of 33.64 \$/GJ, but with the added advantage of negligible SCE of 0.003 kg/kWh of Scenario 1.

4.2.4. Parametric study outcomes

As depicted in Fig. 14, increasing the absorption chiller temperature has a detrimental effect on the system's overall thermodynamic behavior. In particular, the higher temperature lowers the temperature drop of purified vapor during condensation in heat exchanger E-109 and the subsequent expansion in valve VLV-102 that lowers the heat exchanger E-110's capacity to produce chilled water. This performance degradation results in a reduced η_{en} of approximately 61.7%. Moreover, the system experiences higher $\dot{E}x_D$, reaching 4933 kW, which slightly diminishes the η_{ex} to around 53.92%. From an environmental perspective, the SCE and GWP of the system improve, decreasing to 0.0041516 kg/kWh and 0.164 kg/kWh, respectively, while EDEI deteriorates by increasing up to 85.45% due to intensified destruction of exergy. In economic terms, the LCOE and the TUCP rise to 0.295 \$/kWh and 34.24 \$/GJ, as a consequence of reduced energy and exergy outputs. Simultaneously, the NPV decreases to 11.05 M\$, attributed to lower annual revenue generated from diminished cooling production.

In Fig. 15, it can be seen that the growing in E-100 outlet temperature has a negative impact on the system's performance. The higher

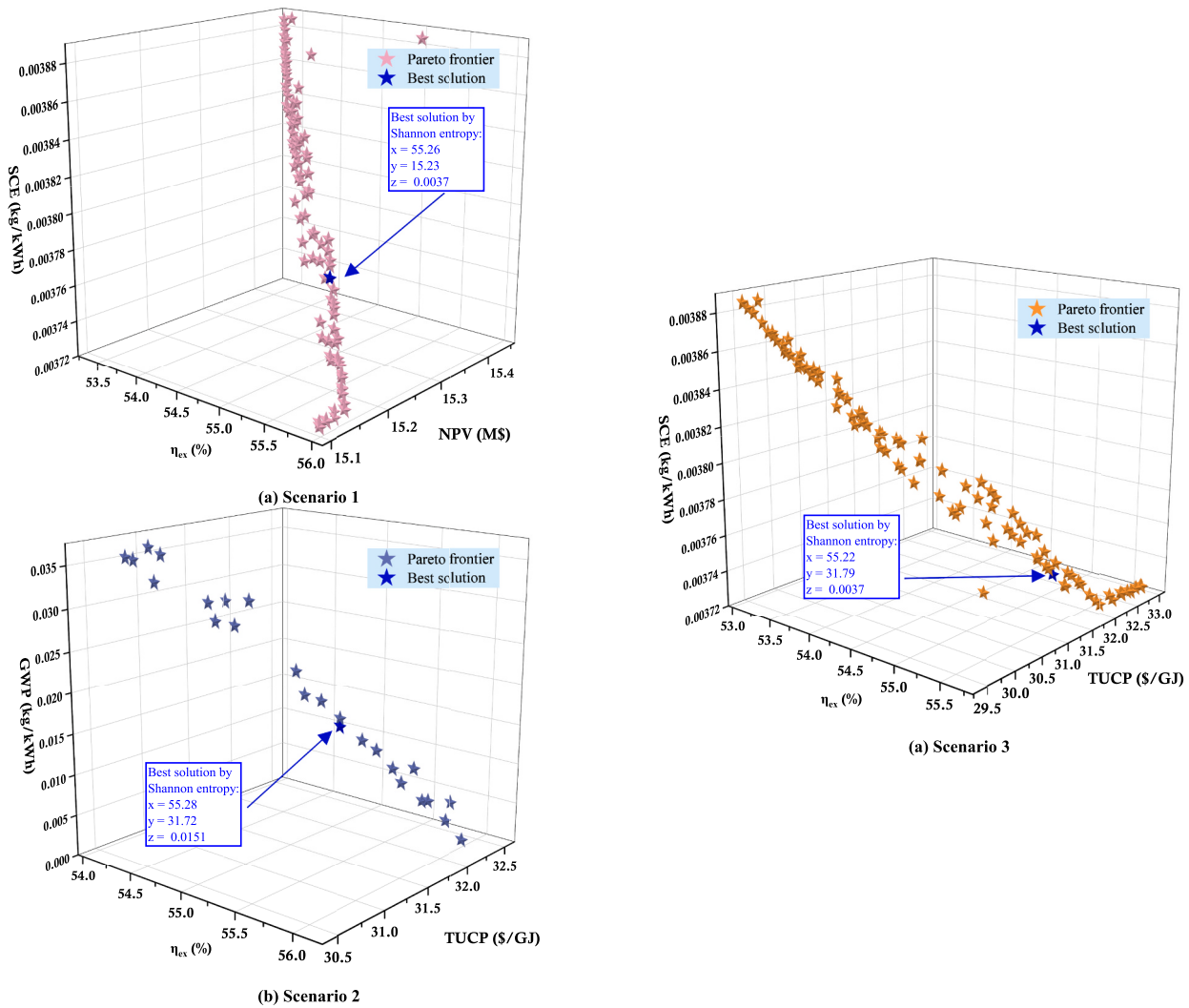


Fig. 23. The outcomes of three-objective optimization via MOCSO algorithm for the modified System II.

temperature lowers heat integration in the steam Rankine though E-100, which results higher utilization of flue gas temperature using E-103. This results lower power and cooling generation from the system, that their combined effects diminish the η_{en} of the system to 61.69%. From an exergy perspective, the system experiences a higher $\dot{E}x_D$ of 4992 kW, which causes a slight reduction in η_{ex} to around 53.38%. In terms of environmental performance, the SCE and GWP exhibit degradation, rising to 0.0038 kg/kWh and 0.199 kg/kWh, meanwhile, the EDEI increases markedly to 87.33%, reflecting the greater exergy destruction and reduced exergy efficiency. Economically, the system also suffers performance setbacks so that the LCOE and TUCP escalate to 0.295 \$/kWh and 34.39 \$/GJ, due to the diminished energy and exergy outputs, while NPV declines to 11.12 M\$, attributed to reduced annual income.

The system's performance is improved by increasing the steam pressure inside the Rankine cycle as shown in Fig. 16. Based on the analysis, greater expansion of the higher-pressure steam fed to turbine T-101 directly boosts power production and raises the η_{en} to 63.43%. On the other hand, reduced irreversibility helps the system from an exergy perspective so that $\dot{E}x_D$ drops to 4912 kW, which results in an increase in η_{ex} to about 54.12%. The environmental performance also improves under this condition so that the SCE and GWP decrease to 0.00414 kg/kWh and 0.168 kg/kWh, respectively, while the EDEI declines to 84.75% due to the lower destruction of exergy. Economically, the system demonstrates favorable outcomes, with the NPV rising to 11.72 M\$

as a result of higher annual income from increased power generation. However, despite the higher output, the LCOE and TUCP still increase slightly, reaching 0.287 \$/kWh and 33.91 \$/GJ, reflecting the balance between improved performance and associated cost implications.

According to Fig. 17, by increasing the K-101 outlet pressure, the system's thermodynamic behavior is changed in negative side. The increased heat utilization of compressed air in heat E-102, which draws more energy from the flue gas, results in less flue gas heat being available for integration with the boiler and steam Rankine cycle, which lowers heating and power generation. This performance deterioration lowers the system's η_{en} to 61.16%. On the exergy side, the system has higher irreversibility, with $\dot{E}x_D$ increasing to 4974 kW, which causes a slight drop in η_{ex} to 53.54%. Economically, the poor performance results in higher production costs, with the LCOE and TUCP rising to 0.298 \$/kWh and 34.28 \$/GJ, while the NPV falls to 11.40 M\$, mainly due to lower annual income from lower power and heating outputs. The environmental indicators also show deterioration under this condition so that the SCE and GWP both rise, and the EDEI reaches to 86.76% as a result of increased destruction of exergy.

By considering Fig. 18, the performance of the system is adversely affected by increasing the turbine T-101 outlet pressure. The analysis reveals that it reduces the steam expansion ratio within the turbine, which lowers the power output of the Rankine cycle and, as a result, lowers the overall power generation of the integrated system, resulting in a reduced η_{en} of 62.57% for system. From an exergy perspective,

irreversibility worsens, with Ex_D increasing to 4971 kW, which slightly reduces the η_{ex} to 53.57%. The environmental performance indicators also deteriorate so that the SCE and GWP increase to 0.0038 kg/kWh and 0.181 kg/kWh, while the EDEI increases to 86.66% due to higher exergy destruction and diminished exergy efficiency. Economically, this condition results in higher production costs, with LCOE and the TUCP rising to 0.291 \$/kWh and 34.26 \$/GJ.

4.2.5. Sensitivity analysis outcomes

Figs. 19 and 20 depict the outcome related to sensitivity analysis of system performance indicators using two complementary approaches. First, the SHAP-based sensitivity analysis provides data-driven rationale for relative design parameter significance, their quantitative role in performance indicators variations [112]. The second, the Morris method evolved Spider plot sensitivity analysis provides graphical representation of performance variations due to variation of parameters with percentage change of 40%, keeping others fixed individually [113].

The results show that the E-100 outlet temperature and the K-101 outlet pressure are the most important factors influencing exergy efficiency, that increasing either of these parameters tends to increase thermodynamic irreversibility, which in turn reduces η_{ex} , while their lower values have a positive effect by increasing system's η_{ex} . As for environmental indicators, the T-101 outlet pressure is the most important factor affecting SCE, and the K-101 outlet pressure is the most important parameter influencing GWP. In both situations, increased pressure values result in higher emissions, which deteriorated environmental sustainability, while operating at lower pressures reduces both SCE and GWP, supporting more environmentally favorable outcomes in line with decarbonization goals. Economically, the TUCP shows a strong sensitivity to E-100 outlet temperature, so that higher temperatures increasing production costs due to reduced power and heating generation, while its lower values result in lower TUCP. Similarly, the absorption chiller temperature is a key factor in determining the system's NPV so that higher temperatures reduce cooling output and annual revenue, which lowers the NPV, while lower values raise the profitability and NPV.

4.3. Second scenario outcomes (System II vs. System I)

Fig. 21 presents a comparison of the NPV for the two proposed systems over a 20-year plant lifetime. System II (methane-geothermal multi-generation) consistently exhibits higher NPV values than System I (methane-based tri-generation), reflecting the economic advantage of integrating geothermal energy and multi-effect desalination. By year 20, System II achieves a final NPV of approximately 14.07 M\$, compared to 11.6 M\$ for System I, indicating that the second system allows a greater return on capital investment while maintaining enhanced multi-generation performance. These results highlight that, relative to System I, the incorporation of geothermal heat not only improves operational flexibility and energy utilization but also significantly enhances the overall economic performance of the plant, confirming the financial viability of the second scenario for long-term deployment.

Table 12 compares key performance, economic, and environmental indicators for System I vs. System II. The modified case (System II) demonstrates notable improvements across almost all metrics. Primary energy savings increase from 44.25% to 52.99%, indicating more efficient fuel utilization. Both energy and exergy efficiencies show modest gains (63.03% to 65.50% and 54.00% to 54.51%, respectively), reflecting slightly better conversion and reduced irreversibilities.

Economically, the modified system incurs only a marginal increase in equipment cost (27.7 → 27.9 M\$) but yields a higher NPV (11.6 → 14.07 M\$), a shorter PBP (8.1 → 7.48 years), and a higher IRR (0.1987 → 0.2106), highlighting improved financial viability. LCOE drops significantly from 0.2897 to 0.1998 \$/kWh, and TUCP decreases from 34 to 32.35 \$/GJ, indicating better economic efficiency.

Environmentally, GWP is substantially decreased from 0.173 to 0.0179 kg/kWh, showing the modified system's superior sustainability performance. Overall, the modified scenario (System II) offers enhanced thermodynamic, economic, and environmental outcomes compared to System I.

Fig. 22 compares the best compromise solutions of the two-objective optimization (minimizing TUCP and maximizing η_{ex}) in terms of System I and System II using MOPSO, MOALO, MOACO, and MOCOSO algorithms, selected via the Shannon entropy method. For both systems, all algorithms yield closely comparable results, indicating stable Pareto fronts. MOCOSO consistently achieves the highest η_{ex} and the lowest TUCP, demonstrating a superior balance between thermodynamic performance and economic cost. Although the performance differences are modest, the repeated dominance of MOCOSO in both systems confirms its higher robustness and effectiveness in handling conflicting objectives compared to the other algorithms.

Fig. 23 illustrates the results of the three-objective optimization of the modified System II using the MOCOSO algorithm, considering exergy efficiency (η_{ex}), economic performance (NPV, TUCP), and sustainability indicators (SCE, GWP) across three scenarios. The 3D Pareto surfaces reveal clear trade-offs among thermodynamic, economic, and environmental indicators, and the Shannon entropy-selected points represent the most balanced solutions in each scenario.

In Scenario 1 (η_{ex} , NPV, SCE), System II achieves an exergy efficiency of about 55.26%, with an NPV of 15.23 M\$, and SCE of 0.0037 kg/kWh, outperforming System I. In Scenario 2 (η_{ex} , TUCP, GWP), System II attains exergy efficiency of 55.28%, a reduced TUCP of 31.72 \$/GJ, and a markedly low GWP of 0.015 kg/kWh. Similarly, in Scenario 3 (η_{ex} , TUCP, SCE), System II maintains η_{ex} = 55.22%, TUCP = 31.79 \$/GJ, and SCE = 0.0037 kg/kWh. Overall, the modified System II consistently exhibits superior thermodynamic, economic, and sustainability performance across all scenarios, demonstrating the effectiveness of MOCOSO in identifying robust, well-distributed optimal solutions for complex multi-criteria energy system optimization.

5. Conclusion

The current study proposed and systematically evaluated advanced carbon-neutral tri- and multi-generation energy systems with an emphasis on deep system-level thermal integration and comparative utilization of alternative heat sources for CO₂ capture. Two distinct but unified integration scenarios were investigated. **System I** represents a highly integrated methane-fueled tri-generation configuration in which a modified gas turbine, recuperative steam Rankine cycle, boiler, and absorption chiller are synergistically combined with a MEA-based CO₂ capture unit for electricity, cooling, heating generation. **System II** extends this architecture into a multi-generation platform by introducing renewable geothermal energy as a secondary heat source to supply the CO₂ capture reboiler and to drive a multi-effect desalination unit, enabling the additional production of freshwater and domestic hot water.

Thorough thermo-enviro-economic analyses, including energy, exergy, exergo-economic, exergo-environmental, and gate-to-gate life cycle assessment, were conducted for both scenarios. In addition, a data-driven multi-objective optimization framework was implemented using XGBoost surrogate modeling, Shannon entropy decision-making, and comparative benchmarking of four advanced metaheuristic algorithms. Plus, sensitivity and parametric analyses further clarified the robustness of the proposed systems and identified the most influential design parameters. The key finding of this research can be summarized as below:

- **System I** achieved simultaneous production of 5702 kW of power, 465 kW of heating, and 141 kW of cooling, with overall energy and exergy efficiencies of 63.03% and 54.00%, respectively, demonstrating effective cascade utilization of fuel energy.

- The integrated MEA-based CO₂ capture unit attained an exceptionally high CO₂ removal efficiency of 98.78%, reducing emissions from 1975 kg/h to 21.47 kg/h, mainly due to stable reboiler heat supply and enhanced absorption conditions.
- From an environmental standpoint, System I exhibited a specific global warming potential (GWP) of 0.173 kg/kWh and specific carbon emission (SCE) of 0.0037 kg/kWh, confirming its strong decarbonization potential relative to conventional fossil-based systems.
- Economically, System I proved viable, with a levelized cost of energy (LCOE) of 0.2897 \$/kWh, a total unit cost of product (TUCP) of 34 \$/GJ, a 20-year NPV of 11.6 M\$, and a payback period of 8.1 years.

Plus, the introduction of geothermal energy in **System II** resulted in substantial performance improvements:

- Primary energy savings increased from 44.25% to 52.99%, while energy and exergy efficiencies rose to 65.50% and 54.51%, respectively.
- System II achieved a significantly higher net present value (NPV) of 14.07 M\$, a shorter payback period of 7.48 years, and a higher internal rate return (IRR) of 0.2106, demonstrating superior long-term economic attractiveness.
- The LCOE and TUCP were reduced to 0.1998 \$/kWh and 32.35 \$/GJ, respectively, reflecting improved economic efficiency through renewable heat integration. Environmental performance improved markedly, with the specific GWP decreasing to 0.0179 kg/kWh, confirming the strong sustainability advantage of geothermal-assisted CO₂ capture and desalination.

Multi-objective optimization results showed that all applied algorithms generated stable Pareto fronts; however, the Multi-Objective Chameleon Swarm Optimization (MOCSSO) algorithm consistently delivered the most balanced solutions across both systems. For System II, three-objective optimization revealed optimal compromise solutions with exergy efficiency of 55.28%, TUCP values as low as 31.72 \$/GJ, and noticeably low GWP of 0.015 kg/kWh, confirming the robustness and effectiveness of the proposed optimization framework.

Despite these promising outcomes, some limitations should be acknowledged. The life cycle assessment (LCA) was limited to a gate-to-gate operational boundary, excluding emissions related to equipment manufacturing, end-of-life recycling, and upstream material production. Moreover, the analysis was conducted under steady-state conditions, and dynamic operation, part-load behavior, and component degradation were not considered.

Future research should therefore extend the present framework toward cradle-to-grave LCA, incorporate dynamic and off-design analyses, and explore alternative low-carbon solvents and renewable heat sources. Experimental validation of key subsystems and real-time optimization under variable demand conditions would further enhance the applicability and scalability of the proposed systems. Overall, this work establishes a scenario-based, system-level integration pathway for next-generation carbon-neutral tri- and multi-generation energy systems, offering valuable insights for sustainable energy transition and long-term decarbonization strategies.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.applthermaleng.2026.130093>.

Data availability

The authors do not have permission to share data.

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