



Thermodynamic analysis of a high-temperature hydrogen production system

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Abstract. Using clean energy resources is considered as a major solution to global warming. Hydrogen is one of the most popular clean and renewable fuels, which has widely been addressed by researchers in different contexts from additive fuel of internal combustion engines to pure feed of fuel cells. Hydrogen production is also one of the most interesting fields of study and extensive effort has been devoted to finding high-performance, fast, and economical approaches in this field. In this study, a novel high-temperature steam electrolyser system with an integrated solar Brayton cycle core is proposed and numerically simulated for hydrogen production. Energy and exergy analyses were carried out to gain better perception of the performance of the system and Rankine and Organic Rankine Cycle (ORC) were integrated with the main core to improve its efficiency. The influences of different parameters such as turbine inlet temperature, inlet heat flux from the sun, and compression ratio as well as the used organic fluid were investigated based on the first and second laws. Results showed the high performance of the proposed system with more than 98% energy efficiency in hydrogen production besides its simplicity of use. The highest exergy destruction occurred when the power generation system absorbed sun heat flux (more than 54%) and the performance of the system could be enhanced by improving the heat absorbing technology.

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1. Introduction

Dependence of the world on fossil fuels for transportation, buildings, and electricity generation has sharply increased since the industrial revolution. Indeed, the life standards have increased as well. However, some concerns, e.g., regarding climate change, global

warming, acid rains, pollution, increase in sea levels, and ozone layer depletion, have also grown alongside [1]. Accordingly, the use of other sources of energy has become more and more vital [2]. Researchers consider hydrogen as a renewable and clean alternative energy resource in different areas from methanol production [3] to its use as a pure/additive fuel in internal combustion engines [4–7]. Although hydrogen abundantly exists on the earth, it can only be found in the composition of other materials. Consequently, hydrogen production has changed into one of the most interesting fields of study and extensive research has been carried out on improving economic efficiency of hydrogen production

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[8–10]. However, more studies are still needed to achieve higher exergy efficiency and thermodynamic analysis of different systems is a proper domain of effort in this regard [11–13].

The use of renewable sources to produce hydrogen can be categorized into two main groups of low- and high-temperature electrolyzing. High-temperature electrolyzers are more efficient than low-temperature ones because of good ion conduction at an elevated temperature [14,15]. However, they require more inlet power and heat. The demanded heat and power by these electrolyzers can be provided through different thermodynamic cycles employing solar [16], wind turbine [17], nuclear [18], and geothermal [19] energy technologies. The solar based system proposed by Ozcan and Dincer [20] overall had 18.8% energy and 19.9% exergy efficiency and they asserted that it could be improved to 26.9% and 40.7%, respectively, employing the heat absorbed by the molten. Balta et al. [21] divided their solar based system into the power generation and hydrogen production sections. They reported that the energy and exergy performances of the Power Generation System (PGS) were 24.79% and 22.36% and of the hydrogen production system were 87% and 88%, respectively. A conceptual design of photovoltaic solar energy conversion was presented by Bhattacharyya et al. [22]. They estimated the efficiency of their proposed thermodynamic and conversion module. Sayyaadi [23] utilized new a setup for dual hydrogen-power generation plant. The nuclear-based High-Temperature Steam Electrolysis (HTSE) proposed by Ozcan and Dincer [24] had 18.6% and 31.35% energy and exergy efficiency and the overall energy and exergy efficiency of the coal gasification based hydrogen production system proposed by Seyitoglu et al. [25] was 41% and 36.5% respectively. Moreover, exergy efficiency of the biogas-based HTSE hydrogen production proposed by Abuşoğlu et al. [26] was 25.83%.

In this paper, a high-temperature electrolyzer is employed for hydrogen production. A Brayton cycle integrated by solar energy is used to provide the electrolyzer with the demanded heat and power. In addition, Rankine and Organic Rankine Cycle (ORC) are utilized to enhance efficiency of the system. In order to compare two working fluids of the ORC, the proposed system is analyzed under the first and second laws to find the best operating condition.

2. System definition

The proposed hydrogen production system has two main parts, namely hydrogen production and power generation. The hydrogen production part is derived from Ref. [27] in which hydrogen is produced via HTSE method. Through this method, the high-temperature

steam is divided into pure hydrogen and oxygen by the received electricity from PGS. The demanded heat is also provided from the waste heat of the PGS. Two heat exchangers are also utilized to use the heat of the separated hot hydrogen and oxygen, as shown in Figure 1. More details on HTSE and the employed heat exchangers are available in [27].

The power generation section consists of three cycles, namely, Brayton, Rankine, and ORC. The demanded power and heat by the electrolyzer are produced through Brayton cycle. In this cycle, air is compressed in a two-stage compressor via and inter-cooler, which cools it down to the ambient temperature. The feedwater to the electrolyzer is pre-heated by the absorption of the inter-cooler waste heat. Then, the compressed air is pre-heated in the solar receiver and more heat is added to achieve the highest feasible temperature due to the erosion of the turbine blades in the combustion chamber. The energy of air is first converted to the power via the turbine and then, absorbed by the pre-heated feedwater to the electrolyzer. Then, the extra energy of air is employed to run Rankine and ORC boilers. Finally, a simple Rankine cycle and an ORC with regenerator are utilized to convert the extra energy of the air to the power. The general characteristics of the integrated system are reported in Table 1.

3. Model description

The equations for the first and second laws are employed for each component to analyze the performance of the integrated system. The required equations are given in this section and the following assumptions are made to simplify modelling:

- All sections (PGS and the electrolyzer) are modeled by Steady-State Steady Flow (SSSF) process;
- The thermodynamic tables are used for the data on air, water, and CO₂ properties;
- Pure methane is used as fuel for the combustion chamber;
- The outflows of the condensers of ORC and Rankine cycle are assumed saturated liquid;
- Air and combustion products are assumed as ideal gases.

3.1. Energy analysis

With the above assumptions, mass conservation and energy equation for each multi-input-multi-output component in the SSSF process [28] can be written as:

$$\sum \dot{m}_e = \sum \dot{m}_i, \quad (1)$$

$$\dot{Q} - \dot{W} = \sum \dot{m}_e h_e - \sum \dot{m}_i h_i. \quad (2)$$

Here, \dot{m} and h are the mass flow rate and enthalpy and

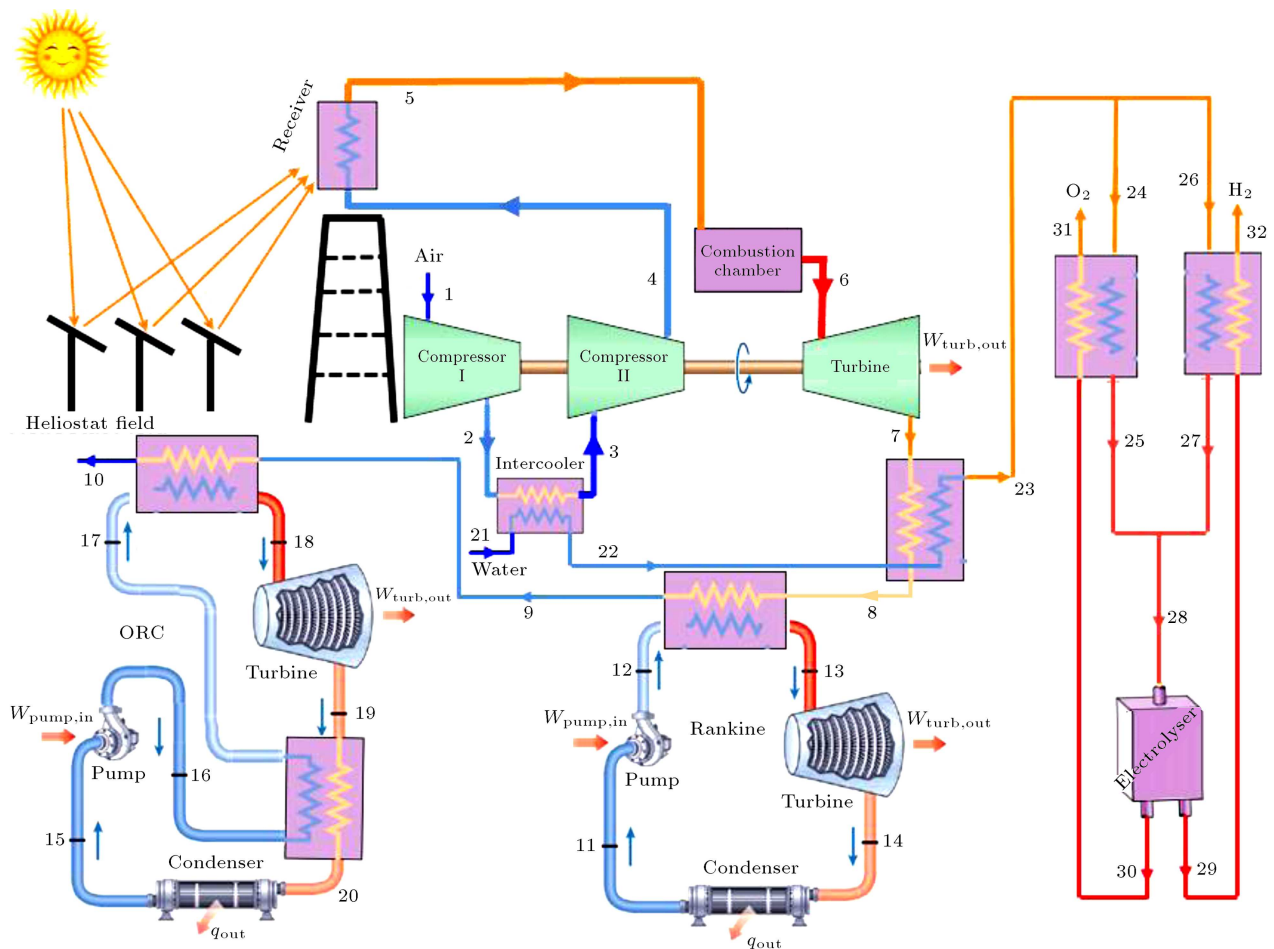


Figure 1. Schematics of the proposed system.

the subscripts i and e refer to inlet and exhaust flows, respectively. The correlations of ideal gas are employed for the Brayton cycle [28]:

$$Pv = R_u T, \quad (3)$$

$$h = C_p T, \quad (4)$$

$$u = C_v T. \quad (5)$$

Here, the pressure, specific volume, temperature, and internal energy of the working fluid are shown by P , v , T , and u , respectively. C_p and C_v refer to the special heat with constant pressure and volume, respectively, and R_u expresses the universal constant of gases. Considering ideal gas as the working fluid of the Brayton cycle, the outside temperatures of compressors and turbine exhaust flows can be written as [28]:

$$\frac{T_e}{T_i} = 1 - \eta_{tur} \left(1 - \left(\frac{P_e}{P_i} \right)^{\frac{k-1}{k}} \right), \quad (6)$$

$$\frac{T_e}{T_i} = 1 - \eta_{comp} \left(1 - \left(\frac{P_e}{P_i} \right)^{\frac{k-1}{k}} \right). \quad (7)$$

In these equations, k is the ratio of special heat coefficients. Moreover, η_{tur} and η_{comp} refer to the isentropic efficiency of the turbine and the compressor, respectively. In case of steam turbines and pumps, characteristics of the exhaust flows can be defined as [28]:

$$\eta_{tur} = \frac{h_i - h_e}{h_i - h_{es}}, \quad (8)$$

$$\eta_{pump} = \frac{h_i - h_{es}}{h_i - h_e}. \quad (9)$$

Here, the index *es* refers to the isentropic operation. All the processes of heat exchangers are assumed isobar and sufficient working pressure of the intercooler is calculated as [28]:

$$P_{intercooler} = \sqrt{P_1 P_4}. \quad (10)$$

The sum of the generated/consumed power by turbines, compressors, and pumps is called net power and is calculated for each cycle. In addition, the ration of the net power to inlet heat is called thermal efficiency. As an example, for the proposed Brayton cycle, we have [28]:

Table 1. General characteristics of the proposed system [21].

Solar tower	
Receiver height	65 m
Number of heliostats	69
Total area of heliostat field	8349 m ²
Brayton cycle	
Working fluid	Air
Turbine isentropic efficiency	0.92
Compressor isentropic efficiency	0.88
Compression ratio	11.2
Turbine power capacity	5670 kW
Rankine cycle	
Working fluid	Water
Turbine isentropic efficiency	0.91
Pump isentropic efficiency	0.88
Turbine inlet temperature	623.15 K
Turbine inlet pressure	3000 kPa
Turbine exit pressure	65 kPa
Turbine power capacity	1020 kW
ORC	
Working fluid	CO ₂
Turbine isentropic efficiency	0.95
Pump isentropic efficiency	0.90
Turbine inlet temperature	453.15 K
Turbine inlet pressure	15000 kPa
Turbine exit pressure	7000 kPa
Turbine power capacity	445 kW

$$\dot{W}_{net} = \dot{W}_{GT} + \dot{W}_{comp1} + \dot{W}_{comp2}, \quad (11)$$

$$\dot{Q}_{net} = \dot{Q}_{receiver} + \dot{Q}_{C.Ch}, \quad (12)$$

$$\eta_I = \frac{\dot{W}_{net}}{\dot{Q}_{net}}. \quad (13)$$

The mass flow rates of inlet fuel, Rankine cycle, the feedwater in the hydrogen production section and ORC can be calculated considering the temperature gradient of the hot side of heat exchangers by assuming adiabatic operations [28]:

$$\dot{m}_{mix} C_{p,mix} (T_6 - T_5) = \dot{m}_{fuel} \eta_{comb} LHV, \quad (14)$$

$$\dot{m}_{mix} C_{p,mix} (T_8 - T_7) = \dot{m}_{water} (h_{22} - h_{23}), \quad (15)$$

$$\dot{m}_{mix} C_{p,mix} (T_9 - T_8) = \dot{m}_{Rankine} (h_{12} - h_{13}), \quad (16)$$

$$\dot{m}_{mix} C_{p,mix} (T_{10} - T_9) = \dot{m}_{ORC} (h_{17} - h_{18}), \quad (17)$$

where η_{comb} and LHV refer to the combustion process efficiency and Low Heating Value of the used fuel, respectively, which are considered 0.98 and 47.13 MJ/kg [29]. In addition, \dot{m}_{mix} and $C_{p,mix}$ are the mass flow rate and specific heat of the combustion products, respectively.

3.2. Exergy analysis

Second-law analysis, as another means of evaluating the performance of a device, can be carried out after performing the first-law analysis of each component and defining thermodynamic properties of each steam. Thus, exergy balance equation is introduced as [28]:

$$\dot{E}x^Q + \sum \dot{m}_i ex_i = \dot{E}x^W + \sum \dot{m}_e ex_e + I, \quad (18)$$

where $\dot{E}x^Q$, $\dot{E}x^W$, ex , and I are exergy transfers due to heat transfer, exergy transfer from work, specific exergy, and destructed exergy, respectively. Total exergy for each steam is divided into thermo-mechanical and chemical exergy as [28]:

$$ex = ex_{tm} + ex_{ch}, \quad (19)$$

$$ex_{tm} = (h - h_0) - T_0(s - s_0), \quad (20)$$

$$ex_{ch} = \sum_{i=1}^N y_i ex_i^{ch} + RT_0 \sum_{i=1}^N y_i \ln(y_i), \quad (21)$$

where s and y_i are entropy and the mole fraction of fluid compositions, respectively, and index 0 refers to the dead state, which is defined for working fluid properties in ambient pressure and temperature. The exergy of fuel is defined by a semi-empirical equation from [30] as:

$$\varepsilon = \frac{ex_{fuel}}{LHV}, \quad (22)$$

where ε is considered close to unity. Exergy transfer by the work and the passed heat from the system boundaries [28] are:

$$\dot{E}x^W = \dot{W}, \quad (23)$$

$$\dot{E}x^Q = \left(1 - \frac{T_0}{T_s}\right) \dot{Q}, \quad (24)$$

where T_s refers to the temperature of heat source. Exergy efficiency, as the more accurate criterion of system operation, is introduced as the division of the achieved to the consumed exergy [28]:

$$\psi = \frac{E_{x_{net}}}{E_{x_i} - E_{x_e}}. \quad (25)$$

For hydrogen production performance analysis, thermal efficiency is defined as the ratio of the LHV of the separated hydrogen from feedwater to the heat entered to the system. For the second-law efficiency, exergy of the separated hydrogen is compared with the inlet exergy:

$$\eta_I = \frac{\dot{m}_{H_2,sep} LHV_{H_2}}{Q_{in}}, \quad (26)$$

$$\psi = \frac{Ex_{H_2,sep}}{Ex_{in}}. \quad (27)$$

4. Results and discussion

Since the proposed system is based on a novel idea, experimental data are not available to validate the results. Thus, each employed cycle is separately validated via given data from a previous study [21], which are shown in Table 2. As indicated, reliability of the generated results by the provided model is at a high level since the model has high accuracy in prediction of the system performance.

After defining the thermodynamic characteristics of each steam, the home-made simulator model can calculate the performance of the proposed system. The thermodynamic characteristics of each steam are reported in Table 3. The overall performance of the system was evaluated using the available data besides the defined equations in the section on model description. The results are briefly given in Table 4. While 7532 kW of the total 8873 kW net power was produced by the Brayton cycle, almost 90% of the total irreversibility was also from this cycle. The first law efficiency of PGS and hydrogen production was 50.7% and 98.3%, respectively.

The performance of the proposed system with the change of Brayton turbine inlet temperature when the other inlet parameters are considered fixed are shown in Figures 2 and 3. The demanded fuel increased by 36.8% to achieve 1600 K while the heat received from the sun had no change. The consumed fuel enhancement rate was greater than the turbine out-power rate. Therefore, the ratio of power to added heat in combustion chamber slightly decreased. Furthermore, irreversibility of the general system increased due to higher heat transfer rate in heat exchangers

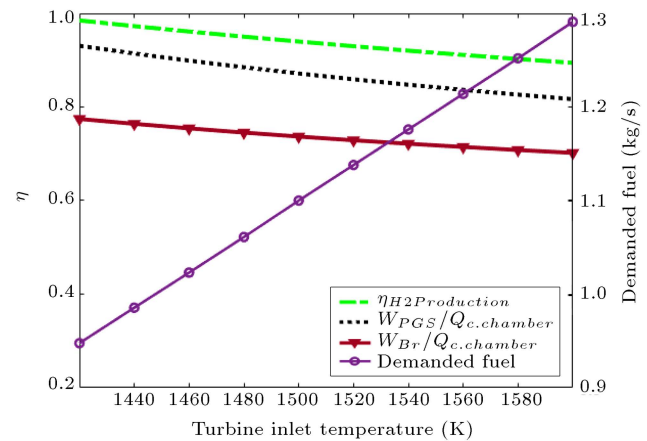


Figure 2. First-law analysis of the proposed system via turbine inlet temperature.

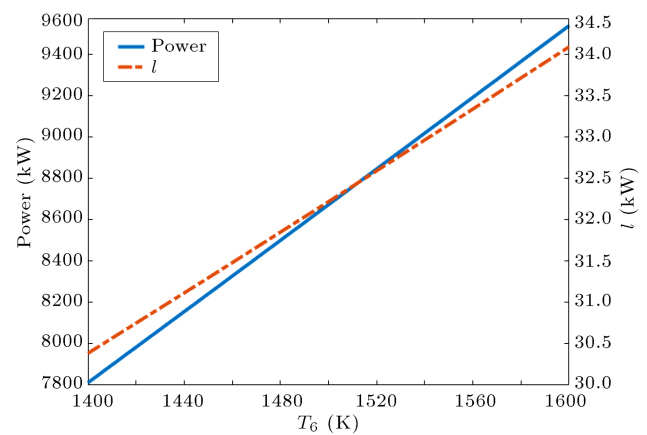


Figure 3. Net power and irreversibility of Power Generation System (PGS) via turbine inlet temperature.

and hydrogen production efficiency decreased by 6% due to the increase in fuel consumption by the rise in turbine inlet temperature. System response to input heat flux from the sun is shown in Figure 4. With fixed turbine inlet temperature, less fuel was needed when the input heat flux increased. Consequently, the

Table 2. Comparison of reference and simulated data.

Cycle	Energy efficiency		Exergy efficiency		Exergy destruction [kW]		Power generation [kW]		$\frac{\dot{m}_{H_2,produced}}{\dot{m}_{H_2,interred}}$ (%)	
	Ref. [21]	Sim. ^a	Ref. [21]	Sim.	Ref. [21]	Sim.	Ref. [21]	Sim.	Ref. [21]	Sim.
Brayton	38.7	38.79	47.71	50.7	206	2321	5670	5681	—	—
Rankine	24.21	24.22	40.19	63.72	1523	1137.2	1020	1015	—	—
ORC	25.28	25.34	40.55	32.52	376	337	445	326.5	—	—
Simple PGS (overall)	24.79	24.79	22.36	27.15	17338	19030	7135	7022	—	—
Simple HTSE (overall)	—	30.98	—	0.399	18130	20163	—	—	66.62	65.43

^aSim.: Simulation.

Table 3. Characteristics of each steam in the proposed system.

State no.	Fluid	T (K)	P (kPa)	\dot{m} (kg/s)	h (kJ/kg)	s (kJ/kgK)	ex (kJ/kg)
1	Air	298.2	101.3	14.24	298.6	5.696	0.0
2	Air	434.9	339	14.24	436.7	5.73	127.9
3	Air	298.2	339	14.24	298.6	5.349	103.3
4	Air	434.9	1135	14.24	436.7	5.383	23102
5	Air	903.6	1135	14.24	937.2	6.159	500.5
6	Air	1523	1135	14.24	1664	6.769	1045
7	Air	833.2	101.3	14.24	858.9	6.762	242.4
8	Air	759.4	101.3	14.24	777.8	6.66	191.7
9	Air	480.7	101.3	14.24	483.5	6.179	40.96
10	Air	391.9	101.3	14.24	393.1	5.971	12.38
11	H ₂ O	361.1	65	1.582	368.5	1.169	24.56
12	H ₂ O	361.4	3000	1.582	371.9	1.169	28.01
13	H ₂ O	623.2	3000	1.582	3115	6.742	1110
14	H ₂ O	361.1	65	1.582	2447	1.169	24.56
15	CO ₂	301.8	7000	9.221	-213.9	-1.433	213.4
16	CO ₂	320.4	15000	9.221	-201.1	-1.433	226.3
17	CO ₂	367.1	15000	9.221	-58.1	-1.011	243.5
18	CO ₂	435.1	15000	9.221	81.55	-0.666	280.4
19	CO ₂	383.4	7000	9.221	33.3	-0.666	232.1
20	CO ₂	303.7	7000	9.221	-109.7	-1.088	214.8
21	H ₂ O	298.2	101.1	0.85	104.8	0.3669	0.0
22	H ₂ O	373.1	101.1	0.85	2418	1.306	175
23	H ₂ O	905.1	101.1	0.85	3776	9.172	1047
24	H ₂ O	905.1	101.1	0.28	3776	9.172	1047
25	H ₂ O	1185	101.1	0.28	4426	9.797	1511
26	H ₂ O	905.1	101.1	0.57	3776	9.172	1047
27	H ₂ O	1185	101.1	0.57	4426	9.797	1511
28	H ₂ O	1185	101.1	0.85	4426	9.797	1511
29	H ₂	1233	10000	0.09	12881	60.77	12151
30	O ₂	1233	10000	0.74	966.3	6.643	895.2
31	O ₂	907	7000	0.74	258.1	5.917	403.4
32	H ₂ +H ₂ O	915	7000	0.09+0.02	3913	51.78	5865

Table 4. Performance of the proposed system.

Parameter	Value
Net power	8873 kW
Net irreversibility	32.65 kW
Consumed fuel	1.14 kg/s
Produced H_2	0.09 kg/s
$\eta_{I,PGS}$	50.7%
η_{I,H_2}	98.3%

ratios of produced power and hydrogen to consumed heat in the combustion chamber increased by 29% and 13%, respectively.

Produced power and efficiency of the Brayton cycle are affected by compression ratio and to investigate its impact on the system performance, it was changed between 8 and 16. In Figure 5, first- and second-law efficiency, produced power, and irreversibility of

the Brayton cycle via compression ratio change are shown. All of them increased by rising compression ratio because of higher power generation rate of the turbine than power consumption rate of the compressor. Irreversibility also increased by 4.5 kW with increase in the mean working pressure of the cycle. Considering Brayton cycle as the main power generation core of PGS, total power increased with Brayton cycle. Indeed, higher temperature gradient of the inter-cooler due to isentropic temperature enhancement in the compressor increased the total irreversibility by 13.9%, as shown in Figure 6.

To investigate the role of working fluid on ORC performance, its energy and exergy parameters were compared employing two different working fluids, namely carbon dioxide (R744) and ammonia (R717), as shown in Figures 7 and 8. In case of using carbon dioxide as working fluid, less net power was achieved

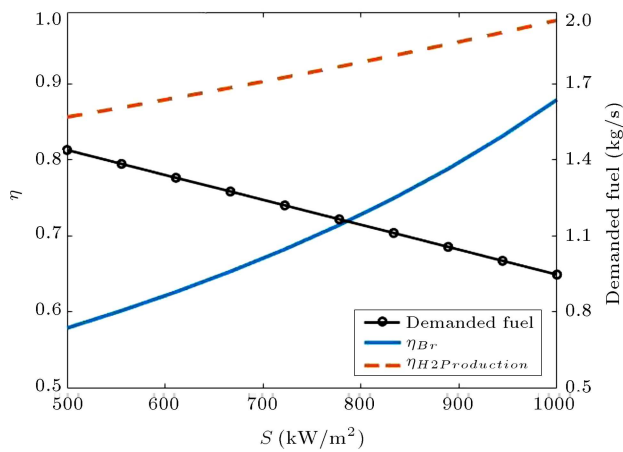


Figure 4. First-law analysis of the proposed system via sun heat flux.

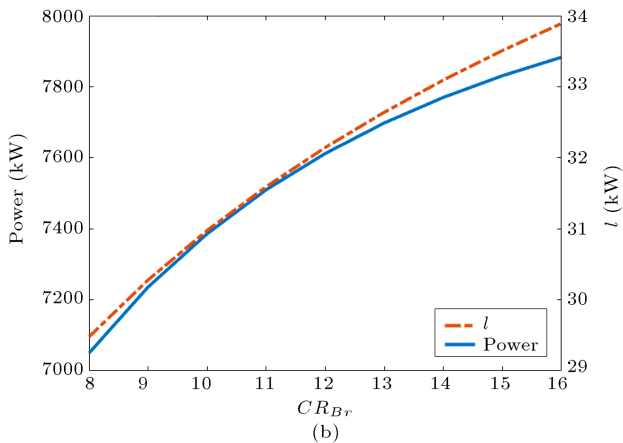
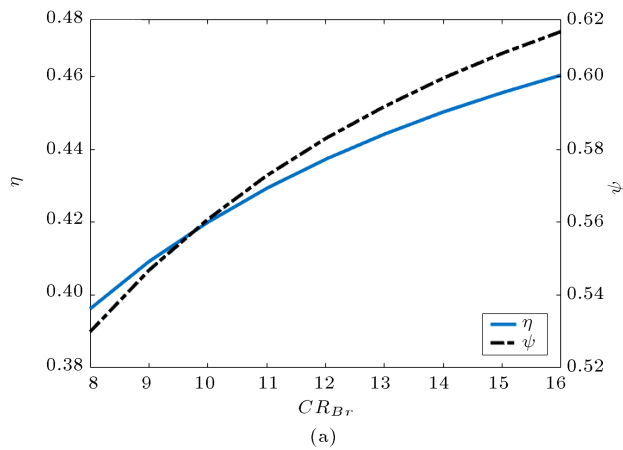


Figure 5. First- and second-law analyses of Brayton cycle via compression ratio.

and irreversibility decreased by 50% in ORC. The synergy of lower power and lower irreversibility led to higher energy and exergy efficiency when carbon dioxide was employed as the working fluid.

5. Conclusion

In this work, a high-temperature electrolyzer integrated

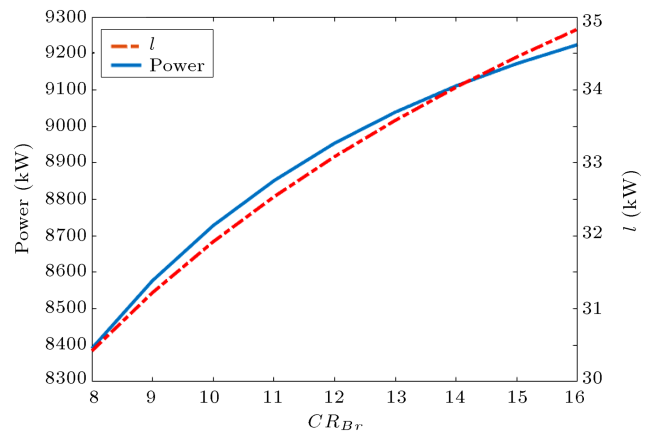


Figure 6. Net power and irreversibility of Power Generation System (PGS) via compression ratio of Brayton cycle.

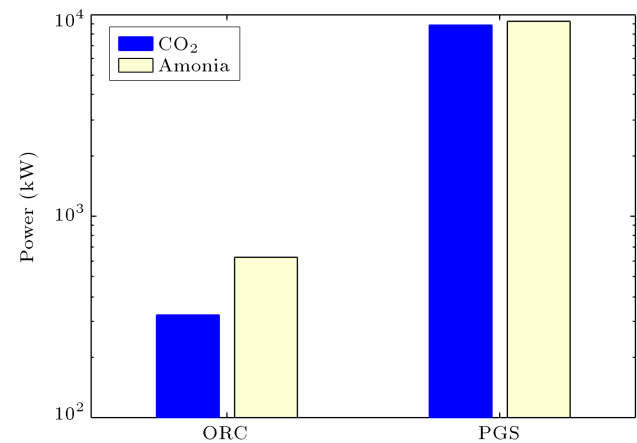


Figure 7. Net power ORC and PGS via ORC working fluid.

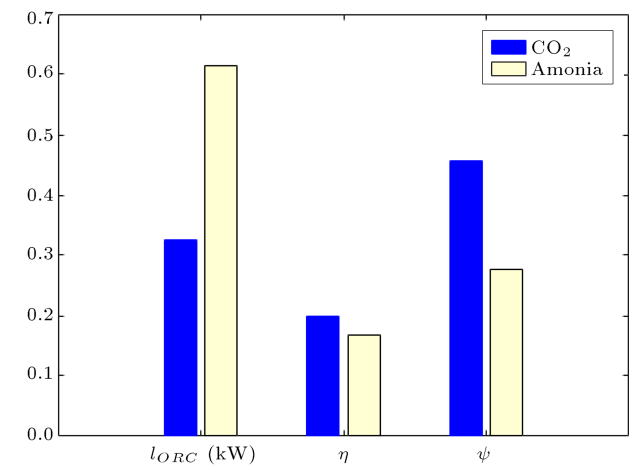


Figure 8. Irreversibility as well as energy and exergy efficiency of ORC via ORC working fluid.

with a Power Generation System (PGS) was proposed and numerically simulated for hydrogen production. The system consisted in a solar-based Brayton cycle developed by Rankine and Organic Rankine Cycle

(ORC). Energy and exergy analyses were carried out and the following main results were obtained:

- The proposed system had more than 98% efficiency in hydrogen production;
- The power generation section had around 50% first-law efficiency;
- The highest exergy destructor section was the solar tower by losing more than 50% of the inlet sun irradiance;
- The proposed Brayton cycle could be more efficient by focusing on reducing irreversibility in the solar tower and combustion chamber;
- Increase in turbine inlet temperature decreased both energy and exergy efficiency;
- ORC produced higher power with lower efficiency by employing ammonia as the working fluid.

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Nomenclature

Abbreviations

HTSE	High-Temperature Steam Electrolysis
PGS	Power Generation System
ORC	Organic Rankine Cycle
LHV	Low Heating Value, kJ/kg
USUF	Uniform-State Uniform-Flow
SSSF	Steady-State Steady Flow

English symbols

C_p	Specific heat at constant pressure, kJ/kgK
C_v	Specific heat at constant volume, kJ/kgK
Ex	Exergy, kJ
ex	Specific exergy, kJ/kg
h	Specific enthalpy, kJ/kg
I	Irreversibility, kW
k	Heat transfer coefficient ratio
m	Mass, kg
P	Pressure, kPa
Q	Heat transfer, kJ
R	Gas universal constant
s	Entropy, kJ/kg.K; Sun irradiance, Wat/m ²

T	Temperature, K
u	Specific internal energy, kJ/kg
v	Specific volume, m ³ /kg
V	Speed, m/s; volume, m ³
W	Work, kJ

Greek symbols

η	First-law efficiency
ρ	Density, kg/m ³
ψ	Second-law efficiency

Subscripts

0	Dead state
1	Primary state
2	Final state
ch	Chemical
comb	Combustion
e	Exhaust
i, in	Inlet
s	Source
sep	Separated
tm	Thermomechanical

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