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Design and optimization of a computer simulation model for green hydrogen production by waste heat recovery from Afyon biogas plant

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ABSTRACT

In this study, a thermodynamic model was designed with the Aspen Plus program and optimized multidimensionally of the Afyon biogas power plant to reduce the unit electricity cost and produce green hydrogen. The model also includes ORC integration to use the exhaust gas energy of the existing power plant. In the model, which includes the whole process from biomass receiving to final electricity production, the plant produces 4000 kW of net electrical power. As a result of ORC integration and optimization, the net electricity production of the plant and ORC were determined as 4625.42 kW and 1215.31 kW, respectively. These values correspond to 0.039 $/kWh unit electricity cost. The power obtained in ORC is stored by producing hydrogen during periods of low electricity demand. For this purpose, ORC power is primarily used to electrolyze H_2S (green hydrogen) released in biogas production. The rest of the power is used in the electrolysis of water. Hydrogen, released in biogas production, is added to the storage process. As a result, approximately 7.447 kg/min of hydrogen is produced at the power plant, costing 0.18 $/kg.

1. Introduction

In 2020, 83% of the world's primary energy consumption is fossil fuels. Energy Council also indicates that it will be 77% in 2040. The energy sector will face fossil fuel scarcity in the future. In addition, population growth and industrial developments have increased the global energy consumption met by fossil fuels. Also, oil and gas extraction techniques are getting more expensive daily. Environmental problems accompany these problems. Using non-renewable energy sources has led to greenhouse climate change, global warming, and gas emissions. These effects have prompted scientists to explore alternative energy technologies. In order to provide energy to a growing population and reduce fossil fuel consumption without harming the environment, switching to a renewable-based energy generation combination is necessary. Biogas can support energy source variations and act as a buffer. Biogas is an important energy source, especially for rural areas, and its other name is green energy. It is a clean energy source that can easily replace fossil fuels and is easy to control. It is mostly (more than 60%) burned in combined heat and power (CHP) to obtain electricity and heat [1-6].

Biogas is an important renewable biofuel produced by the anaerobic digestion of organic wastes such as sewage, animal manure, agro-industrial wastes, landfills, domestic solid waste, and wastewater sludge. In addition to generating heat and electricity in cogeneration systems, it can be used to improve the content of biogas. The gas composition depends on different parameters but generally consists of 35-75% methane, 25-65% carbon dioxide, 1-5% hydrogen, and small amounts of ammonia, water vapor, halides, and hydrogen sulfide. An environmentally friendly fuel feature is that the crops absorb some of the carbon dioxides during biogas production. The upper and lower calorific value of biogas containing 50-75% methane by volume varies between 22-30 MJ/m^3 and 19-26 MJ/m^3, respectively [1, 3, 7-9]. About 40% of the biogas energy is converted to electricity, while about 25% is used to heat the digester. The rest is emitted to the atmosphere as waste heat with exhaust gases. Waste heat units can be used for waste heat recovery. However, waste heat recovery must be economically justified; therefore, a

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thermo-economic optimization should include the entire waste heat recovery unit. This model should be sized correctly for realistic investment costs [3].

Organic Rankine Cycles are generally used for power generation from low-temperature heat sources. They are important alternatives to reduce costs and emissions. At the same time, it creates another alternative as a bottom cycle for the recovery of waste energy in medium and large-scale CHP plants. This technology has advantages such as simple structure, convenient applicability, and user-friendliness over the traditional steam Rankine cycle and is ideal for using medium-low temperature heat sources (<350 ºC). ORC uses organic working fluids; Isobutane is a typical working fluid for temperatures below 200 ºC, while toluene is generally used at higher welding temperatures. ORC applications have been studied on other fluids such as n-pentane, ethanol, R-11, R-123, HFE7100, iso-pentane, benzene, p-xylene, ammonia, cyclohexane, etc. [10-12].

Many studies have been carried out on cogeneration systems regarding thermodynamics and thermoeconomics.

Holik et al. (2021) proposed a thermo-economic optimization model to exploit the waste heat of a two-engine biogas power plant via the Rankine and Organic Rankine Cycle. With the application of the model, the efficiency of the power plant, which was 66.7%, increased by 2.97% with the Rankine Cycle. The payback period of the investment is 6.8 years, and the electricity cost is determined as 0.0419 $/kWh [3].

Baccioli et al. (2019) performed a thermo-economic analysis of ORC integration in a biogas power plant with a 600 kW micro gas turbine in Italy. In the model they developed, it was observed that 77% energy recovery was achieved, and the payback period of the ORC modification was less than 6 years [13].

Gholizadeh et al. (2020) designed a biogas-fed trigeneration system for electricity, cooling, and freshwater production and optimized it exergo-economically for different working fluids. As a result of optimization, a 2.58 % increase in net electricity, 22.69% in cooling load, 14.04% in TGOR (trigeneration-based gain-output-ratio), and 13.26% increase in exergy efficiency was obtained with toluene. The unit cost of the trigeneration system has decreased by 6.71% [14].

Gholizadeh et al. (2019) integrated a gas turbine cycle into the bi-evaporator electric/cooling cogeneration system and analyzed the power plant thermodynamically with the EES program. The cooling load of their proposed system is 505.2 kW; on the other hand, the net electricity it can produce is 1168 kW, and its energy and exergy efficiencies are 54.54% and 36.83%, respectively as a result of integrating the system with the gas turbine cycle increased energy and exergy efficiency by 67.3% and 19.15%, respectively [15].

Gholizadeh et al. (2019) made the feasibility of a biogas-powered gas turbine cycle with ORC. They performed thermodynamic and thermo-economic analyses to estimate system performance and cost. As a result of the analysis, the net electrical power, energy efficiency, exergy efficiency, and total product cost are 1368 kW, 41.83%, 38.91%, and 17.2 $/GJ, respectively [16].

Lu et al. (2022) proposed a new strategy to increase a biogas energy plant's energy efficiency and economic effectiveness. The study consists of 4E and sensitivity analyses. According to simulation results, the plant's thermal efficiency increased from 38% to 46%. The developed system reduces CO_2 emissions by 5100 tons per year. The dynamic payback period and the net present value of the system are about 9.1 years and 4.5 M$, respectively [17].

He et al. (2023) designed a multi-generation system powered by biogas and produced hydrogen, analyzed and optimized thermodynamic, thermoeconomic, and economic. According to thermodynamic analysis results, the system produces 108.7 kW power and 888.7 kW cooling load, respectively; it also produces 703.3 kg/h hydrogen by integrating the steam reforming method and purification process into the system. The energy and exergy efficiencies of the system were also calculated as 31.51% and 31.14%, respectively. The thermoeconomic analysis results show that the total product cost is 16.23 $/GJ [18].

Zhou et al. (2023) proposed a method for a biogas cogeneration system that is powered by biogas and generates electricity and cooling with recovered heat from liquefied natural gas (LNG). The cogeneration system was investigated in terms of thermodynamic, exergoeconomic, environmental, economic, and multi-objective optimization. According to thermodynamic analysis, the developed system produces 1864 kW of electricity and 424.1 kW of cooling power. It has also 80.4% energy efficiency and 41.24% exergy efficiency. According to thermoeconomic analysis, the system has 10.07 $/GJ for the unit's overall product cost for a selling price of 0.27 $/kWh for cooling and 0.06 $/kWh for electricity. Finally, according to environmental analysis, the cogeneration system reduces amounts of CO_2 released from 6091 kg/MWh to 3913 kg/MWh after optimization [19].

Gargari et al. (2019) performed the multi-criteria optimization of the power plant in terms of energetic, exergetic, exergoeconomic, and environmental aspects. As a result of the optimization, the system has a 123.59 MW cooling capacity, 0.73 MW heating capacity, 280.35 MW net power, 18.14 kg/h distilled water, and 0.2432 kg/h hydrogen production capacity. In this case, the system's energy efficiency is 72.75%, the exergy efficiency is 50.21%, the unit product cost is 6.79 $/GJ, and the environmental penalty cost rate (environmental penalty cost rate) is determined as 168 $/h [4].

Abusoglu et al. (2021) investigated the potential of district heating (DH) based on biogas, heat, and electricity production of a wastewater treatment plant. The study consists of district heating scenario I (DH Scenario I) based on excess biogas storage and exhaust gas and district heating scenario II (DH Scenario II) based on exhaust gas and power output using all biogas. According to the analysis results, with the district heating scenario I, 458 houses can be heated, and the natural gas needs 1112 houses with the same heating load; with district heating scenario II, the heating load of 755 houses can be met with waste heat. In addition, payback periods for district heating scenarios I and II are calculated as 2.5 and 2 years, respectively [8].

Cao et al. (2021) proposed a biogas-fed seasonal gas turbine cycle in terms of thermodynamics and economy. They designed and optimized a cogeneration system for electricity/heating and electricity/cooling, with the bottom cycle independent of the season. As a result, energy efficiency, exergy efficiency, and cost of products were calculated as 79.2%, 45.6%, and 21.7 $/GJ for summer, and 70.7%, 37%, and 17.6 $/GJ for winter, respectively [7].

This study presents a realistic model to reduce the unit cost of electricity produced by a biogas power plant operating in Afyon, make exhaust gases less harmful, and use waste exhaust gas energy. The current power plant has a power of 4 MW and does not utilize exhaust gas waste heat. In this regard, the model proposes the integration of an ORC into the power plant and optimizing the combined system. With the proposed model, the power plant produces green hydrogen by electrolysis of water by producing extra electricity with waste heat.

2. Afyon Biogas Plant and Operating Principle

The Afyon biogas plant is given in Figure 1. Afyon Biogas Plant produces biogas by decomposing 150,000 tons of organic vegetable and animal waste annually in an airless environment with anaerobic fermentation technology. The power plant has an electrical power of 4000 kW. It produces odorless, solid organic fertilizer with high organic matter content, free from gases and other components which harm the air and soil, after hygiene process of raw material. The plant solves this problem by transforming it into renewable energy and organic fertilizer production with high organic matter content. So, 177,000 tons of carbon emissions annually are prevented as well as disposing of animal and vegetable origin wastes, a important environmental problem. Solid and liquid organic fertilizer production are 20,000 and 80,000 tons/year, respectively.

The operating principle of the Afyon biogas plant is given in Figure 2. The biomass received by the plant is mixed with water in the circulation tank. It is then sent to the reactor to be digested. Biogas is released as a result of digestion. The biogas is passed through a bio cleaner and a dryer to turn into pure methane.

On the other hand, atmospheric air is compressed by a compressor. The exhaust gas heats the compressed air in the preheater and is ready for combustion. In the combustion chamber, methane gas and air perform the combustion reaction. Exhaust gas from the combustion reaction runs the turbine, producing electricity. The shaft power produced is converted into electrical power by the generator. Exhaust gas is passed through the air preheater due to its high energy. Finally, the exhaust gas is sent to the reactor to increase the temperature. In this study, the exhaust gas drives an ORC before the reactor. So, the power plant efficiency increases, and the electricity produced becomes cheaper. While the electricity produced in the existing power plant is transferred to the grid, The electricity produced in the ORC is used to produce hydrogen. In this way, hydrogen energy can be used when needed.

The hydrogen separated from the biogas in the bio cleaner is sent to the hydrogen tank, and hydrogen sulfide separated from the biogas in the bio cleaner is sent to electrolysis. The power required for electrolysis is supplied from the ORC. The remaining ORC power is used in the electrolysis of water. The exhaust gas driving the ORC then heats the water to increase efficiency in water electrolysis. Finally, the exhaust gases are sent to the reactor and released into the atmosphere.

3. Analyzes and Optimization

3.1 Thermodynamic Analysis

The thermodynamic analysis is done to see the thermodynamic performance of the power plant and to be a preliminary step towards optimization with thermoeconomic analysis. The power plant is optimized by using thermodynamic and thermoeconomic equations. The main equations given below were used for thermodynamic analysis. The electrical power, ORC power, and net electrical power of the plant are:

$$\dot{W}_{electricity} = \dot{W}_{turbine} - \dot{W}_{compressor} \tag{1}$$

$$\dot{W}_{ORC} = \dot{W}_{ORC\,turbine} - \dot{W}_{pump} \tag{2}$$

$$\dot{W}_{Net\,electricity} = \dot{W}_{electricity} + \dot{W}_{ORC} \tag{3}$$

Specific physical exergy and physical exergy are:

$$ex_{phy.n} = h_n - h_0 - T_0\left(s_n - s_0\right) \tag{4}$$

$$\dot{E}x_{phy.n} = \dot{m}_n ex_{phy.n} \tag{5}$$

Chemical exergy is:

$$\dot{E}x_{ch.n} = \sum_{k=1} x_k \bar{ex}_{ch._k} + \bar{R}T_0\left(\sum_{k=1} x_k \ln^{x_k}\right) \tag{6}$$

So, total exergy is:

$$\dot{E}x_n = \dot{E}x_{phy.n} + \dot{E}x_{ch.n} \tag{7}$$

Figure 1. Afyon biogas plant [20].

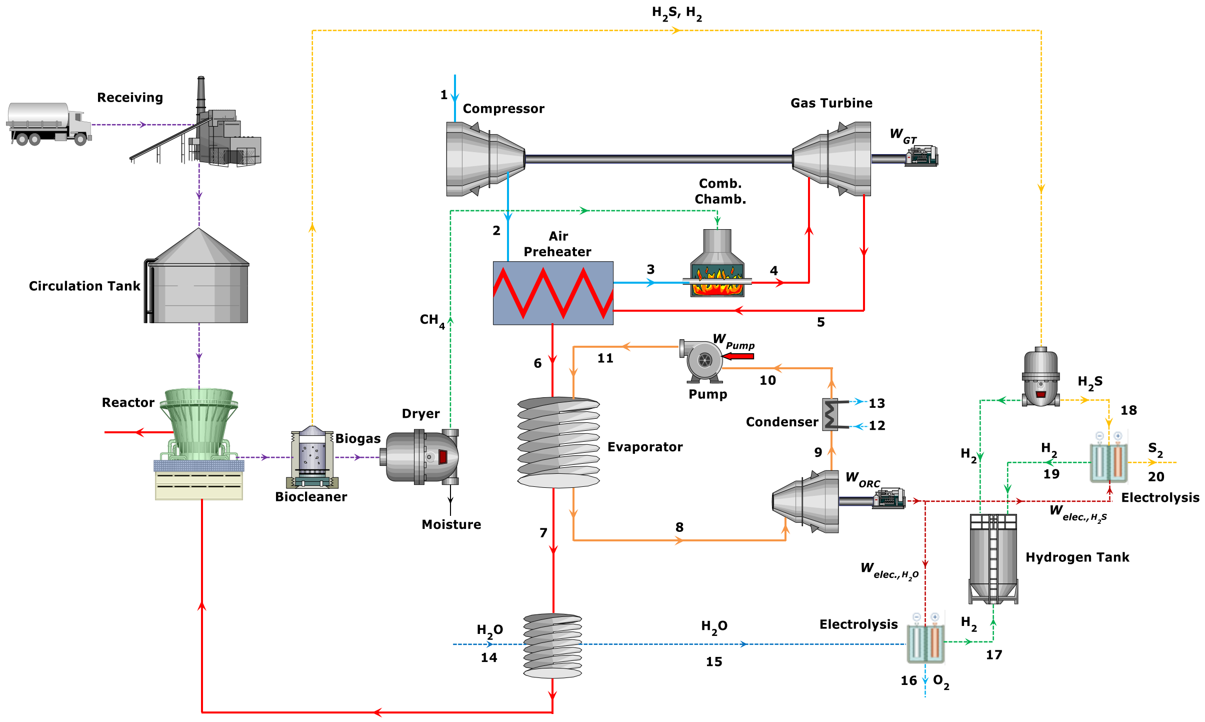

Figure 2. The operating principle of the Afyon biogas plant.

In this case, energy and exergy efficiencies are where *HV* is the heating value of biogas:

$$\eta_{energy} = \frac{\dot{W}_{Net\ electricity}}{\dot{m}_{biogas} HV_{biogas}} \tag{8}$$

$$\eta_{exergy} = \frac{\dot{W}_{Net\ electricity}}{\dot{E}x_{biogas}} \tag{9}$$

In addition, the equations used in the electrolysis are as follows:

$$\Delta G + T\Delta S = \Delta H \tag{10}$$

$$\eta_{energy} = \frac{HV_{H_2} \dot{m}_{H_2}}{\dot{W}_{electricity}} \tag{11}$$

$$\eta_{exergy} = \frac{\sum \dot{E}x_{products}}{\dot{W}_{electricity} + \dot{E}x_{reactants}} \tag{12}$$

3.2 Thermoeconomic Analysis

Thermoeconomic analysis is done to calculate the unit costs of the products of the plant. Exergetic data obtained in the thermodynamic analysis are used in thermoeconomic analysis. Each exergy is based on a specific cost to establish an economic relationship between the plant's products, equipment, heats, works, fuel, operating and maintenance, etc. The capital recovery factor, total cost rates, and unit costs must be calculated. The main equations used in thermoeconomic analysis are as follows. Here *CRF*, *i*, and *n* are capital recovery factors, interest rate = 15% and plant life = 20, respectively.

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1} \tag{13}$$

C_k, φ and $\dot{Z}_k$ are equipment purchasing cost, operation and maintenance factor and total cost rate, respectively.

$$\dot{Z}_k = \frac{C_k (CRF)\varphi}{(n \times 3600)} \tag{14}$$

The exergy cost rate equations are as follows:

$$\dot{C}_w = c_w \dot{W} \tag{15}$$

$$\dot{C}_q = c_q \dot{E}x_q \tag{16}$$

$$\dot{C}_i = c_i \dot{E}x_i = c_i (\dot{m}_i ex_i) \tag{17}$$

$$\dot{C}_e = c_e \dot{E}x_e = c_e (\dot{m}_e ex_e) \tag{18}$$

A cost balance for a system component can be written as follows:

$$\sum_i \dot{C}_{i,k} + \dot{C}_{q,k} + \dot{Z}_k = \sum_e \dot{C}_{e,k} + \dot{C}_{w,k} \tag{19}$$

3.3 Optimization

The main factor in formulating an optimization problem is the selecting of independent variables which characterize design options. In selection of variables, there is a need to consider entire critical variables which affect the cost-effectiveness and performance of system, not select variables that are too detailed or unimportant, and distinguish between independent variables whose values may vary. For example, in a preliminary design, it is generally optional to consider each system component's design details [21].

In this study, optimization was made in the Aspen Plus program to maximize the CHP net electrical power and minimize unit electricity cost in a multidimensional way. Aspen Plus is chemical process optimization software used by the biochemical industries to design, operate, and optimize safe and profitable manufacturing facilities. Aspen Plus changes many parameters to increase economic performance. These parameters can be the increase or decrease of pressures and temperatures or the addition or removal of equipment in the workflow. With the change made, the economic performances of the existing and changed processes are compared. If the modified process does not meet the optimization goal, the process is changed again. Optimization parameters and operating limits are given in Table 1 [22].

4. Results and Discussion

To facilitate interpretation of the results, Figures 3, 4, and 5 represent key findings from the optimization process. Figure 3 shows the effect of the change in AFR on net electricity generation. According to the figure, the power produced by the plant increases with the increase of AFR. However, with the increase of AFR, the exhaust gas (T_6) temperature that drives the ORC unit decreases. For this reason, the working fluid Toluene cannot be evaporated in the ORC unit because the T_6 temperature drops excessively at AFR values greater than 70. Therefore, this area is a risky area for ORC business fluid. The optimum AFR has been determined as 70 to avoid power loss in the ORC unit.

Table 1. Optimization parameters and operating limits.

Parameter	Operating Limits
Air-fuel ratio (AFR)	50 – 70
Rise of pressure(r_p)	6 – 15
T_3 (K)	750 – 825

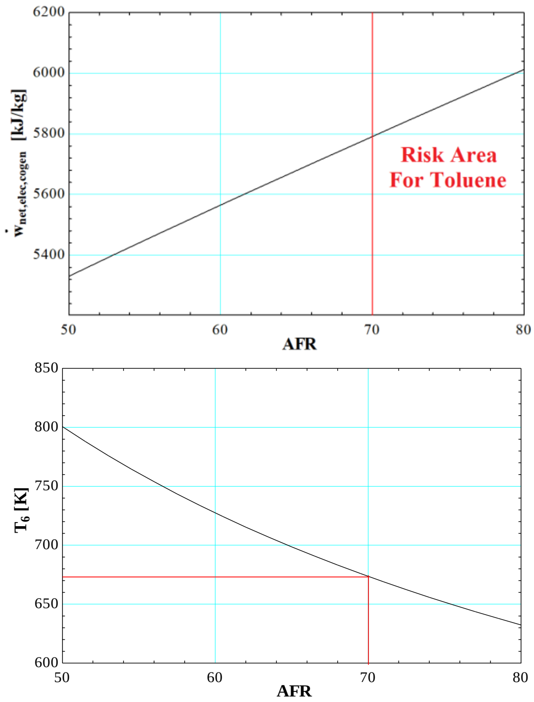

Figure 3. The effect of the change in AFR on net electricity generation.

Figure 4 shows the effect of the change in rp on net electricity generation. In Figure 4, r_p of 9.393 is the compressor's critical value; at higher r_p values, the net power produced from the plant decreases. Therefore, the compression ratio is determined as the optimum r_p.

Figure 5 shows the effect of the change in T_3 temperature on the net power produced by the plant. According to the figure, as the T_3 temperature increases, the power of the plant increases. However, as the T_3 temperature increases, the exhaust temperature T_6 decreases. As in Figure 3, since the exhaust gas temperature of T_6 drops too much at levels of T_3 higher than 780 K, the working fluid (Toluene) cannot be evaporated in the ORC. Therefore, T_3 temperatures above 780 K are risky for the working fluid in the ORC cycle. Therefore, the optimum T_3 temperature is determined as 780 K.

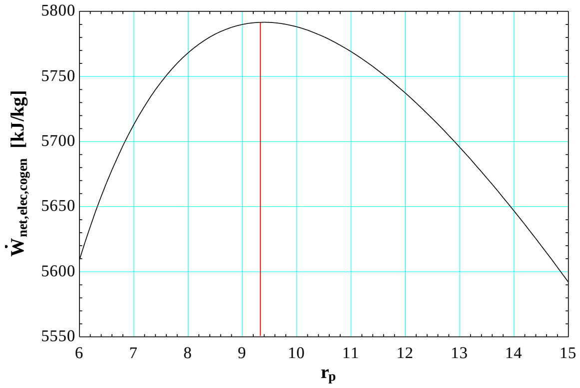

Figure 4. The effect of the change in r_p on net electricity generation.

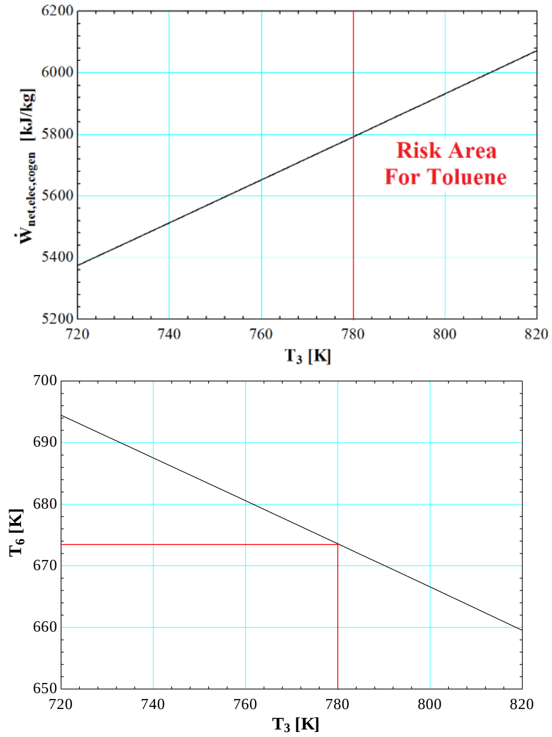

Figure 5. The effect of the change in T_3 on net electricity generation.

Figure 6 shows the Afyon biogas plant designed and optimized in Aspen Plus. The upper left side of the figure represents biogas production from biomass. The upper right side shows the electricity production of an existing plant. The released exhaust gases drive the ORC at the bottom right side, producing ORC power. On the lower left side, the electrolysis of water is seen. The light green lines in the middle of the figure represent hydrogen storage.

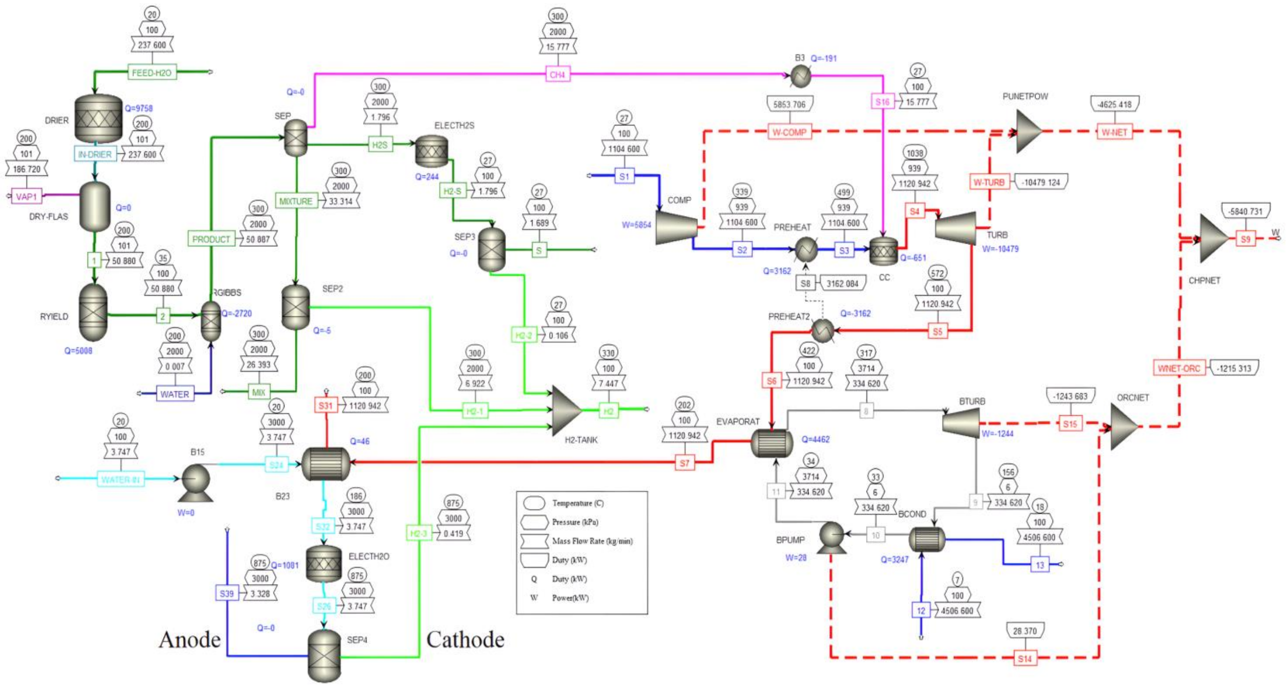

Figure 6. The model designed and optimized in Aspen Plus of Afyon biogas plant.

The figure shows that 5840.73 kW of total power can be produced in the plant. 4625.41 kW of total power is used for electricity generation. Also, 71.86 kW of the 1215.31 kW of power produced in ORC is used at electrolysis of H_2S to produce 0.106 kg/min green hydrogen because if H_2S is not separated from biogas, it damages equipment [23]. The remaining 1095.14 kW ORC power is used at electrolysis to produce 0.419 kg/min hydrogen. In addition, 6,922 kg/min of hydrogen released during biogas production is stored in a hydrogen tank. Therefore, the final hydrogen production is 7.447 kg/min. According to thermodynamic analysis, the energy and exergy efficiency of the plant were calculated as 42% and 36.81%, respectively.

According to thermoeconomic analysis, the cost of unit electricity produced by the plant, which was optimized, was calculated as 0.039 $/kWh. The unit costs of hydrogen obtained from the electrolysis of H_2S and water electrolysis were obtained as 1.42 $/kg and 2.85 $/kg, respectively. The unit cost of hydrogen released in the biogas production process is 0. Therefore, the average hydrogen unit cost is 0.18 $/kg.

5. Conclusions

This study designed a 4000 kW Afyon biogas power plant model to produce cheaper electricity, release less harmful exhaust gas to the environment, and use waste exhaust gas energy. Then, the model was analyzed in terms of thermodynamics and thermoeconomics. The critical results of the study are as follows:

- To use the energy of waste exhaust gas, an ORC was integrated into the power plant, and the combined plant was optimized multi-dimensionally.
- In this way, the power of the plant was increased, and the unit electricity cost was reduced. Reducing unit electricity cost also reduces unit hydrogen cost.
- Generating electricity by utilizing the energy of the exhaust gas ensures that less energetic exhaust gas is released into the atmosphere. In this way, less harm is done to the environment.
- The electricity produced in ORC is stored by hydrogen production when electricity demand is low. ORC power is not used directly in water electrolysis to produce hydrogen. It is first used in H_2S electrolysis to remove H_2S, a harmful component with corrosion for the fuel injection system, and released during biogas production. It is also an advantage that the power required for the electrolysis of H_2S is less than that required for the electrolysis of water [24]. The remaining ORC power is used in the electrolysis of water.

Declaration

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article. The author(s) also declared that this article is original, was prepared in accordance with international publication and research ethics, and ethical committee permission or any special permission is not required.

Author Contributions

M.K. wrote the introduction chapter, and M.A. designed the model, carried out analyses, and formed methodology, formulation, and conclusions. C.Y checked up on analyses, grammar, and content of the entire study.

Nomenclature

AFR	: Air-fuel ratio
$\dot{C}$	: Exergy cost rate ($/h)
C_k	: Equipment purchasing cost ($)
ch	: Chemical
CHP	:Combine heat and power
CRF	: Capital recovery factor
ex	: Spesific exergy (kJ/kg)
$\dot{E}x$	: Exergy (kW)
G	: Gibbs free energy (kJ/kmol)
h	: Spesific enthalpy (kJ/kg)
HV	: Heating Value (kJ/kg)
H_2S	: Hydrogen sulfide
i	: Interest rate (%)
n	: Plant life (year)
ORC	: Organic rankine cycle
phy	: Physical
r_p	: Rise of pressure
s	: Specific entropy (kJ/kgK)
S	: Entropy (kJ/K)
T	: Temperature (ºC or K)
$\dot{W}$	: Power (kW)
$\dot{Z}_k$	: Total cost rate ($/h)
η	: Efficiency (%)
Δ	: Change
$\sum$	: Summation symbol
φ	: Operation and maintenance factor
4E	: Energy, exergy, economic and environmental

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