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Hybrid Hydrogen production: Application of CO₂ heat pump for the high-temperature water electrolysis process

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Abstract. Hydrogen is considered an energy vector which ensures a pivotal role in the energy market in near future. As a subsequent, the need to provoke novel technologies and investigate the potential layouts rising from hybridization remains on the shoulder of research literature. The current work investigates the potential role of the supercritical CO₂ heat pump to contribute to hydrogen production inside a hybrid energy system. The case study is a generic biogas power plant characterized by the combination of diverse hydrogen production technologies such as water electrolysis and the reforming process. Water electrolysis takes place through high (SOEC) and low-temperature(AEC) The role of the heat pump unit is defined to operate between these two technologies to recover heat losses and transfer them to high-temperature electrolysis. The performance of the CO₂ cycle in the presented hybrid energy system is simulated via MATLAB SIMULINK and the effective indicators to improve its performance have been carried out. In the end, the result of the simulation shows a production rate of 19.27 kgH₂/h. Furthermore, thanks to heat recovery the total thermal efficiency increases by 80%. It also reveals that the heat pump unit operates with COP in the range of 4.5 – 3.3 based on pressure ratios providing temperature in the range of 151-184 °C by fixing the cold sink input temperature and pressure at 70 °C, 75 bar respectively.

1. Introduction

The energy market will face a rational transition within the upcoming years [1]. Energy systems will have to radically change their structure to integrate 100% renewable generation [2]. This is due to rapid climate changes, especially in recent decades and also the depletion of fossil fuel resources which are considered primary resources until now. Adding to that, the increasing energy demand, all together obligates governments to adopt more environmentally friendly and effective alternatives to change the current situation. Among all solutions, hydrogen, in particular, has gained progressive attention and is marked as the ‘future fuel’ [3]. In contrast with fossil fuels, hydrogen is not a fuel actually but an energy carrier with high energy density [4]. Green hydrogen is produced through renewable resources and reduces greenhouse emissions. As of today, the application of hydrogen is divided into three main categories: transport, more specifically hydrogen fuel cell vehicles [5]; building by blending it into the existing natural gas network (H₂NG), [6] or synthesis of natural gas SNG [7]; power generation, where hydrogen acts as an energy carrier to store excess renewable energy generation (power to power PtP system) [8]. The injection of hydrogen into the gas grid leads to increase energy savings in natural gas end-uses [9]. The hydrogen production market is dominated by biogas reforming technologies which produce 76% of the global rate. On the other hand, hydrogen production from water electrolysis due to its simplicity in practice is among the interesting solutions. However, its share remains less than 0.1%. Although water electrolysis has been around for several decades, in particular the Proton exchange membrane (PEM) and alkaline (AEC) [10], a new line of research in the recent decade has been formed based on high-temperature electrolysis. Such technology can guarantee higher efficiency and are suitable for plants with excess thermal generation. Solid Oxide electrolysis (SOEC) is a promising High-temperature technology with an efficiency range of 74-81% and requires steam of at least 150 °C at 3 bar as an input [11].



CO₂ is a natural non-toxic and inflammable refrigerant. It has a critical temperature of 304.13 K and 73.75 bar pressure. The concept of trans critical CO₂ HP has been already studied in the literature [12]. Due to its thermodynamic properties, it is considered a feasible solution for building applications mostly to provide domestic hot water up to 70 °C [13]. In such a system, the refrigerant at high pressure in the condenser experience no phase change and the heat transfer takes place only through sensible heat. As a consequence, instead of a condenser, it is called gas cooler.

The supercritical CO₂ (sCO₂) cycle has been studied in power cycles deeply as a working fluid in the Rankine cycle, the internal combustion engine (ICE) and nuclear engineering [14]. However, due to its thermodynamic properties, it can be applied inside a heat pump unit in very high-temperature circumstances.

The current framework presents an application of CO₂ heat pump integrated with PtG technologies to improve the water electrolysis efficiency by recovering heat losses related to the joule effect. The water electrolysis is fed by a set of ICEs characterized with power and thermal co-generation. The thermal power is used completely for the biogas reforming process. The CO₂ thermodynamic cycle is designed to operate between low and high-temperature water electrolyzers conditions. As it can be seen in figure 1, SOEC is characterized by thermal requirement as well as power consumption. The heat transfers toward the SOEC direction recovering discharge thermal power from AEC. Due to the criteria of the system that dictates the operational condition, CO₂ remains at a supercritical state throughout its loop. The layout of the power plant is created and simulation is carried out inside the MATLAB SIMULINK environment.

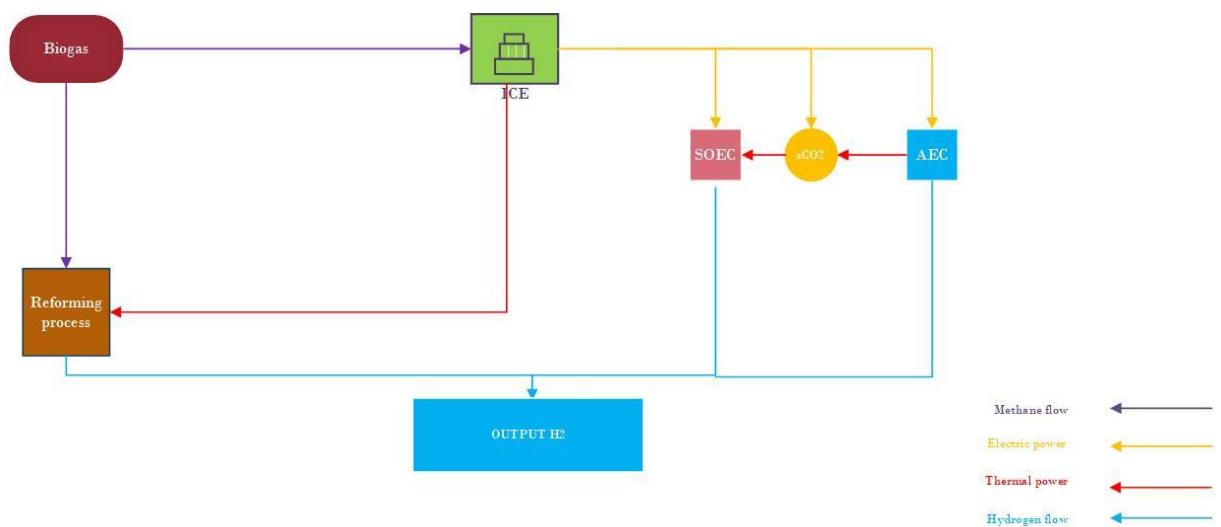


Figure 1. Diagram of the hybrid energy system to produce green hydrogen

1.1. The thermodynamic cycle of the sCO₂ Heat Pump

Figure 2 illustrates the working principle of sCO₂ HP. As it can be seen, the condenser and the evaporator are replaced with ‘gas cooler’ and ‘gas heater’ respectively since in these heat exchangers, heat transfer take place only via sensible heat. An internal heat exchanger unit is placed to recover wasted heat from the gas cooler to increase the temperature of compressor input. The minimum operational criteria for running the cycle in an ultra-critical state should be kept at 31 °C and 73.75 bar. To assure such a set point, the system is designed with low pressure at 75 bar and a minimum temperature of 40 °C which is the input characteristic of gas heater. The hot sink of the heat pump exchanges heats for steam generation at 150 °C and a 3.5 bar SOEC unit which is required for SOEC input. To meet such criteria, the input flow of the gas cooler should provide at least 180°C to make the heat transfer inside the gas cooler feasible. The alkaline electrolyzer (AEC) exchanges the heat needed

for the cold sink. In such a way, the heat loss due to the joule effect in AEC is recovered in the HP system. The working temperature of AEC is 75 °C with an electrical efficiency of 63%.

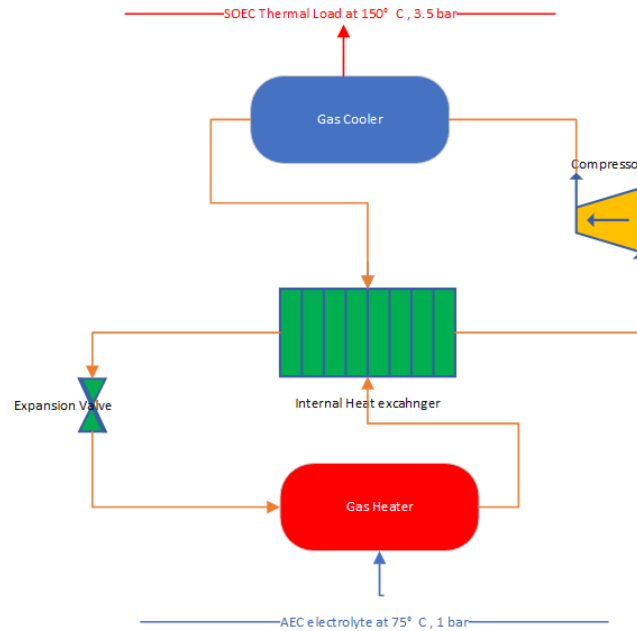


Figure 2. The basic principle of sCO₂ HP cycle

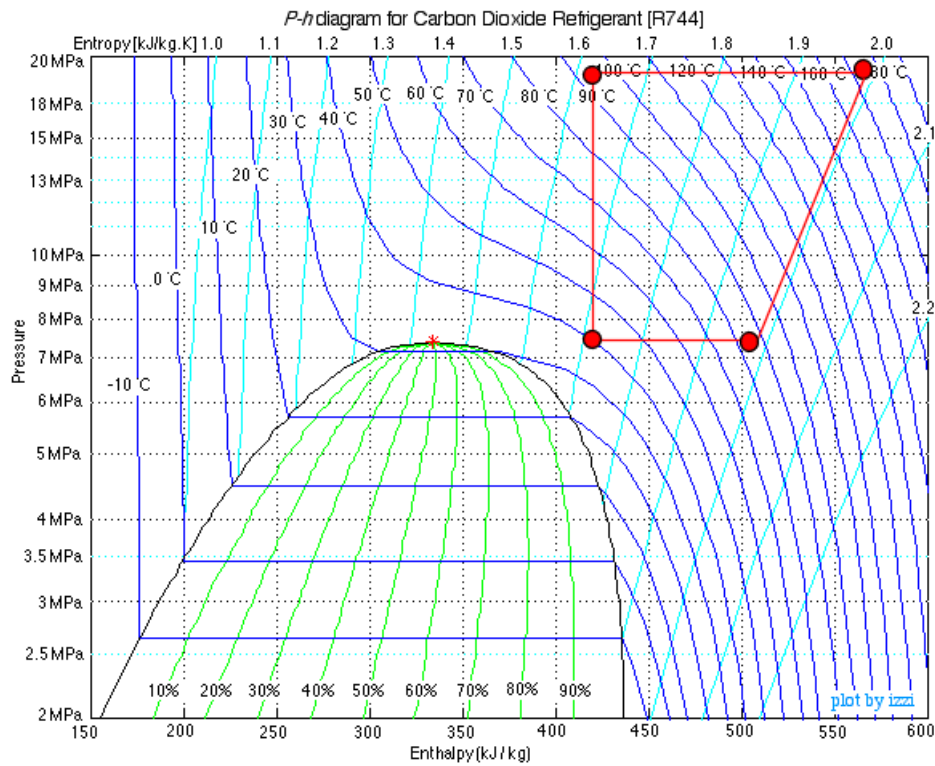


Figure 3. P-h diagram of designed sCO₂ HP

2. Methodology

Table 1 reports the main characteristics of the hydrogen production plant that has been imported for the simulation part. The power plant is characterized by a set of ICE engines fueled with biogas to generate both power and thermal. Thanks to the sCO₂ HP all the heat recovered from ICE engines can be used for the reforming process to increase the production rate. AEC electrolyte exchanges heat with the cold sink of the heat pump. In such a way, the cold sink is characterized by temperature profile at 70 °C and 1 bar pressure. The biogas profile has been used for this simulation assuming with 60% vol methane and about 30% vol CO₂. For this study, a commercial ICE model of JENBACHER J312 gen-set models is assumed with $\eta_{el} = \%40.2$ and $\eta_{th} = \%45$.

Table 1. main characteristics of the biogas power plant used for simulation

Component	measure	unit
BIOGAS flow rate	300	Nm ³ /h
Electric generation	381.4	kW _{el}
Thermal discharge	424.8	kW _{th}
SOEC size	75	Nm ³ /h
SOEC efficiency %	74	
AEC size	14	Nm ³ /h
AEC efficiency%	63	
Reforming	126	Nh ³ /h
Steam flow rate	86	kg/h

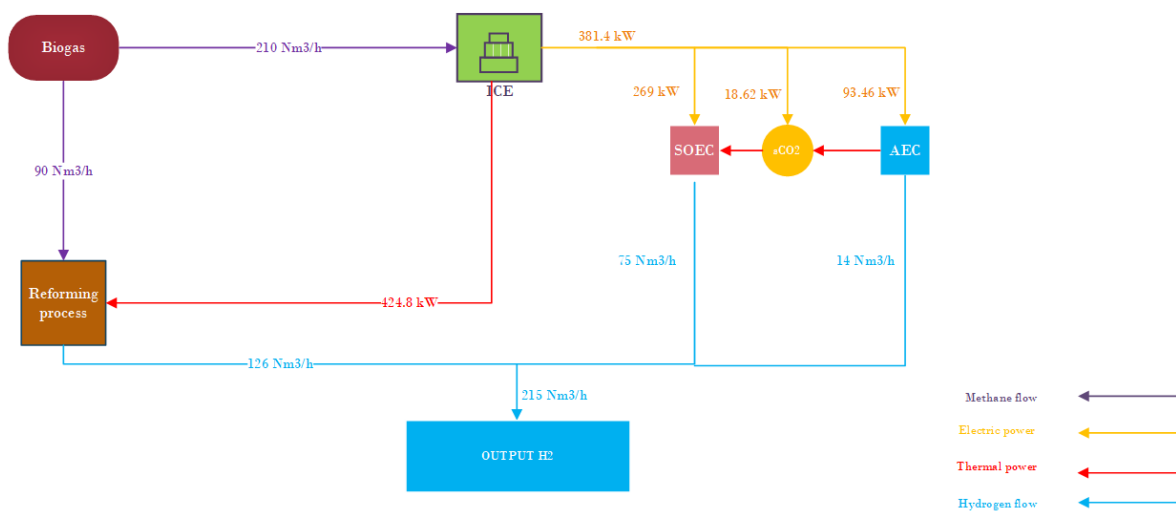


Figure 4. Energy balance of the hybrid energy system

The biogas that flows in the plant is divided into two branches. %70 vol is supplied to the combustion engine and the rest is used for the reforming section. The reforming part is sized to consume almost all of the thermal generation available from CHP. Power generated by ICE is used for both SOEC and AEC units and also for feeding the sCO₂ HP unit. Figure 4, illustrates the energy balance of the hybrid energy system based on the results of the simulation.

During simulation part, the isentropic efficiency is assumed 0.7 and for heat exchangers, the effectiveness is fixed to 0.7. Boundary conditions of the SOEC and ACE dictate temperature set points for hot and cold sink inside sCO₂ HP. Hence, the ideal efficiency of performance (COP) based on the Carnot formula can be evaluated as follow:

$$\eta_{\text{carnot}} = \frac{T_H}{T_H - T_C} = \frac{423}{423 - 343} = 5.28 \quad (1)$$

The actual COP, however, can be obtained based on heat load and input work of the HP unit which is brought in equation 2:

$$\eta_{\text{actual}} = \frac{Q_H}{W} \quad (2)$$

3. Results and discussion

The results of the simulation show the potential H₂ production of 215 Nm³/h with a Levelized cost of Hydrogen (LCOH) equal to 3.95 €/kgH₂. To operate at the nominal power rate of the SOEC device, sCO₂ HP is needed to provide 85 kg/h of steam at 150 °C 3.5 bar. Assuming 75°C is the exhausted temperature of AEC, more than 80% of discharged thermal power can be recovered. Table 2, reveals the optimum design parameters for the sCO₂ HP unit. Under mentioned conditions, a total COP of 3.37 is reachable.

Table 2. The main results of the optimized sCO₂ HP system

Parameter	Measure	Unit
COP	3.37	-
Hot sink size	78	kW
Gas cooler pressure	200	Bar
Cold sink size	30.7	kW
Gas heater pressure	75	Bar
Compressor size	18.6	kW

Due to the meaningful difference between upstream and downstream pressure in the expansion device in figure2, the temperature profile drops rapidly below the critical point causing phase change in such device. To address such an issue, a mid-pressure at 120 bar is considered to avoid temperature drops below 40°C. In this way, after the expansion process the fluid remain at 39.98°C very close to the design set point. In addition to that, the isentropic expansion taking place in such a device release 47.9 kW of useful work which is recovered via a shaft to decrease compression input power. One of the practical parameters to determine the COP of the system is the pressure of the gas cooler. As reported in figure 5, increasing upstream pressure starting from 160 bar has a negative impact on COP due to huge fluctuation in over critical state. However, due to insufficient output temperature and design considerations regarding gas cooler, an effective heat transfer cannot take place if the output temperature drops below 180°C. As a consequence, the upper pressure is set to 200 bar to assure temperature requirement despite the fact that COP is not optimal in this case.

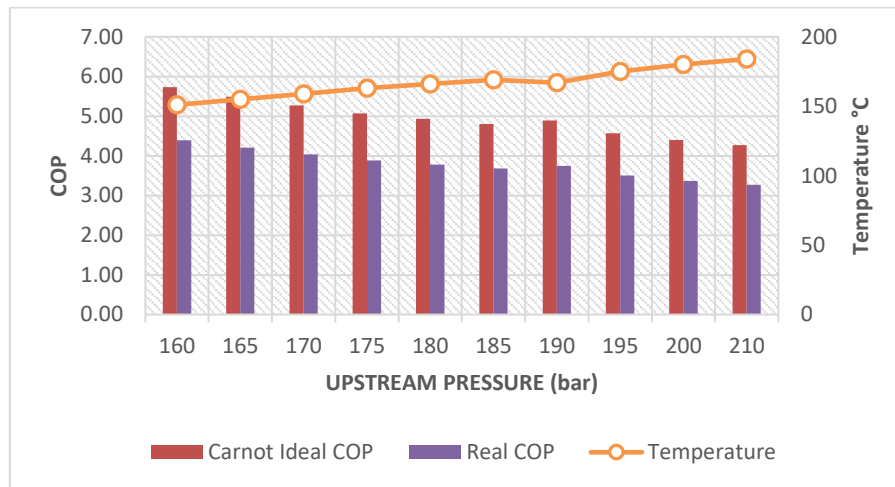


Figure 5. UPSTREAM impact on COP and output temperature

During the simulation, internal heat exchanger effectiveness inside the heat pump is considered constant. Such component is able to recover discharged heat from gas cooler. Another helpful sensitivity analysis is performed on the impact of heat exchanger effectiveness on the overall performance of the heat pump. As a consequence of increasing the effectiveness, the regeneration temperature increases and provide higher temperature gas flow for the expansion device. In this situation the shaft work increases and recover more of the compressor portion. Such results are reported in figure 6 which describes the relation between regeneration temperature in the internal heat exchanger and the overall COP of the device.

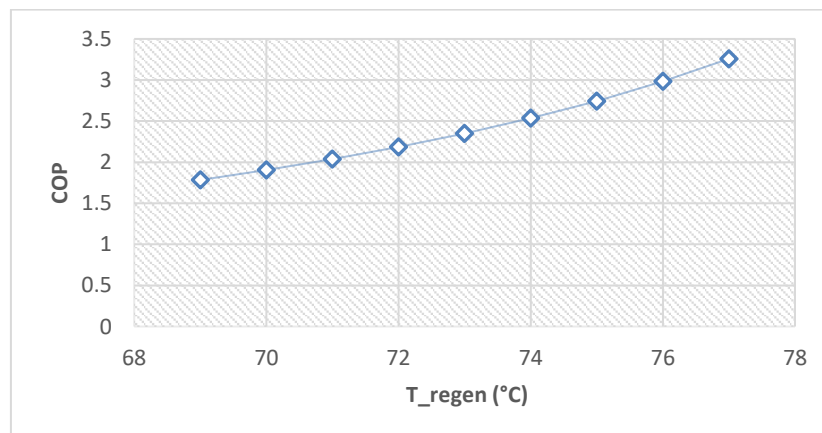


Figure 6. The impact of regeneration temperature in the internal heat exchanger and overall COP of the sCO₂ HP

Conclusion

This study presented an unconventional application for CO₂ heat pump cycle coupled with water electrolysis technologies in order to improve the overall efficiency of AEC. The case study was a biogas-fueled power plant characterized with power and thermal co-generation. In addition to water electrolysis, the reforming process taking place by redirecting thermal power of CHP unit. CO₂Heat pump operates in ultra-critical condition, transferring heat between AEC and SOEC. The design parameters are set to generate steam at 150 °C recovering heat loss from AEC at 70 °C. Results of the simulation suggest the improvement in AEC overall efficiency to %84.6 from %63 initially. with production rate at 85 kg_{H2}/h. In other words the advantage of defining sCO₂ HP in such a way is twofold:

- To respond the heat requirement of SOEC cutting the necessity of an external heat resource

- Improving overall thermal efficiency by recovering discharged heat and reusing it inside an thermodynamic cycle

The sCO₂ HP could reach COP as high as 4.3 however due to temperature set point and boundary conditions of the system, higher pressure with lower COP is set in order to increase as much as possible the output temperature.

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