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Waste-heat upgrading from alkaline and PEM electrolyzers using heat pumps

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ABSTRACT

The use of waste heat from electrolysis can significantly increase process efficiency. Alkaline and PEM electrolyzers, the most mature technologies, produce low-temperature waste heat. Most studies focus on using this waste heat for low-temperature applications like district heating. Alternatively, this waste heat can be upgraded to a temperature that can be usable in the chemical industry, e.g., for steam generation. The combination of an alkaline electrolyzer with a heat pump has been recently investigated to supply both hydrogen and medium-temperature heat. Optimizing electrolyzers for both hydrogen and heat production (combined design) has been shown to have advantages over optimizing for hydrogen only and upgrading the waste heat a posteriori (separate design). However, the effects of electrolyzer pressure and hydrogen compression were not considered, and it remains unclear if similar benefits apply to PEM electrolyzers. This work further analyzes the combined system (i.e., electrolyzer with a heat pump) by including hydrogen compression and comparing alkaline and PEM electrolyzers. The results show that designing with waste-heat utilization in mind benefits both alkaline and PEM at low and high pressures. The combined design allows up to 10% cost reduction and up to fourfold reduction in CO_2 emissions compared to the separate design. However, this benefit is constrained by the maximum achievable current density, particularly for PEM. Despite this limitation, the combined system can effectively supply hydrogen and heat across various energy price scenarios, making it a promising solution for hydrogen supply and industrial electric heating.

Keywords: Hydrogen, Electric heating, Energy, Modelling, Optimization

INTRODUCTION

Waste-heat recovery from alkaline and PEM electrolyzers has been widely studied for low-temperature heat applications (below 100°C), like district heating [1]. However, upgrading electrolyzer waste heat to meet medium-temperature heat demand (e.g., up to 200°C) is less explored, despite recent advancements in heat pump technologies that enable reaching these temperature levels [2]. Moreover, waste-heat utilization is usually added a posteriori after optimizing the electrolyzer for hydrogen production only, which may limit its benefits.

In our previous work [3], we recently explored the advantages of designing an atmospheric alkaline electrolyzer for waste-heat utilization, optimizing for both hydrogen and heat production. This new design approach provided further benefits over using the waste heat a posteriori. Additionally, upgrading waste heat to higher temperatures via heat pumps was found to be preferable over direct use at lower temperatures (e.g., district heating) when heat at both temperatures is required.

However, this previous study did not consider the effects of electrolyzer pressure or the integration with downstream processes: In most industrial applications, hydrogen is required at high pressures (e.g., up to 250 bar for chemical synthesis [4]), requiring a compression step and thus increasing cost and energy demand. Moreover, the same analysis should be extended to PEM electrolyzers, another well-established technology that is drawing increasing interest thanks to its potential for flexible operation.

In this work, we thus further investigate the potential of combined systems to supply both hydrogen and medium-temperature heat. To address the aforementioned shortcomings, we analyze the impact of electrolyzer operating pressure, incorporate hydrogen compression, and compare alkaline and PEM electrolyzers.

SYSTEM DESCRIPTION

The combined system consists of three main units, i.e., a water electrolyzer, a multi-stage compressor with intercooling and a heat pump. The electrolyzer is composed of 26 modules, each one capable of producing 72 kg/h of hydrogen [3]. The hydrogen is subsequently compressed to the required pressure in the multi-stage compressor. Finally, a closed-loop compression heat pump is used to upgrade the electrolyzer waste heat to a higher temperature level. Potential working fluids for achieving the target temperature lift include CO_2, argon, and air.

Such a combined system is able to supply around 1.9 t/h of hydrogen at 75 bar (suitable for methanol production [4]) and heat at 120°C (capable of producing low-pressure steam [2]), thus being an alternative to other electric heating technologies, such as direct electric boilers or air-source heat pumps.

For low-pressure (LP) electrolysis (alkaline and PEM at 1 bar), a multistage compressor with 5 stages is used, whereas for high-pressure (HP) electrolysis (PEM at 30 bar), a single-stage compressor is used. Intercooling to 35°C is considered between stages and before and after the compression step.

METHODOLOGY

Model

The backbone of the mathematical model is based on our previous work [3], which includes the polarization curve of an alkaline electrolyzer, the thermal model of the electrolyzer stack, and the efficiency-based model of different electric heating technologies (heat pump and direct electric boiler). The heat pump, operating at 40% of the maximum COP (i.e., Carnot cycle), achieves COP values ranging from 2.2 to 5.2.

For this work, the polarization curve [5] and Faraday efficiency [6] of a PEM electrolyzer and a multi-stage compressor model based on a fixed isentropic efficiency per stage are added. The molar enthalpies and entropies are computed using data from the CoolProp library [7]. Therefore, the effect of the pressure is captured in the electrolyzer and the compression stage.

Performance evaluation

The performance is evaluated according to two indicators: the levelized cost of hydrogen (LCOH) and the net CO_2 emissions ($NetCO_2$).

The LCOH (Equation (1)) evaluates the total hydrogen production expenses over the system's lifetime (20 years) considering revenue from heat sales. Electrolyzer investment costs are taken from Cooper et al. [8], and replacement costs at the end of the tenth year are considered. Electricity and heat prices are based on the average EU-27 prices (2016-2020) [9]. The rest of model parameters are taken from our previous work [3].

$$\mathrm{LCOH} = \frac{\mathrm{CAPEX}+\sum_{j=1}^{N}(\mathrm{OM}+\mathrm{OPEX}-\mathrm{SALES})\cdot(1+i)^{-j}}{\sum_{j=1}^{N}(m_{\mathrm{H_2}})\cdot(1+i)^{-j}} \qquad (1)$$

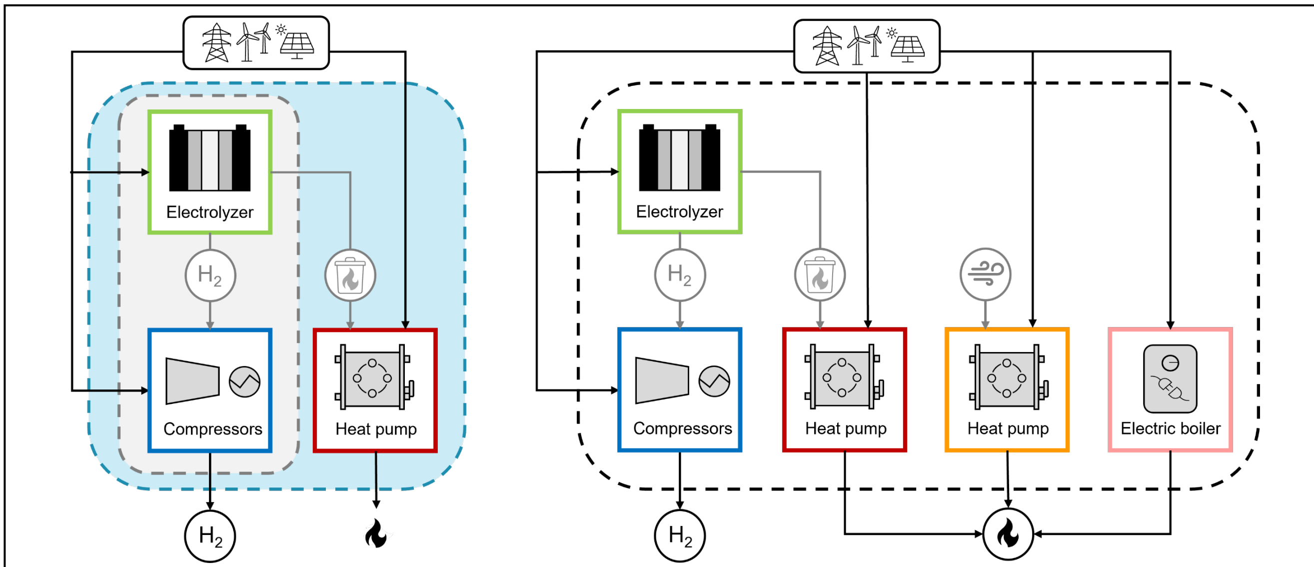

Figure 1. Design of the combined system (left), i.e., electrolyzer with a heat pump, using a separate design (gray) and a combined design (blue), and superstructure diagram of the hydrogen and heat supply network (right). The indicated areas refer to the system boundary considered in the optimization. The circled outputs are fixed.

The $NetCO_2$ (Equation (2)) accounts for the emissions due to electricity consumption of the different units *u* (i.e., electrolyzer, compressors, etc.) and the emissions avoided due to the heat output from electric heating technologies (i.e., heat pump and direct electric boiler), which is assumed to replace heating via natural gas.

$$\mathrm{NetCO_2} = \frac{\mathrm{Em_{ele}}(\sum_u P_u) - \mathrm{Em_{gas}}(\sum_u Q_u)}{m_{H2}} \quad (2)$$

For simplicity, the cooling requirements in the compression unit are excluded from the evaluation as they are small compared to those of the electrolyzer (up to 14% of the waste heat). However, the higher temperature level of the heat from compressor intercooling (140-150°C) makes it a potentially valuable additional heat source, which could further enhance system efficiency.

System design and optimization

We compare the conventional separate design of the combined system, i.e., a posteriori coupling (see Figure 1 left, gray box), with the combined design approach that explicitly incorporates waste-heat utilization (blue box). In both design approaches, we optimize the system for both cost and emissions.

Additionally, we use a superstructure optimization problem to determine the optimal hydrogen and heat supply network, considering various electric heating alternatives, namely air-source heat pumps and direct electric boilers (see Figure 1 right). A hydrogen-to-heat demand ratio of one is considered, where the hydrogen energy content is computed using the higher heating value (HHV).

The electrolyzer optimization variables and the main model parameters are given in Table 1 and Table 2, respectively. Note that the COP of the heat pump is determined by the electrolyzer operating temperature and the sink temperature [3].

Table 1: Electrolyzer optimization variables.

Variables	Alkaline	PEM
Temperature	50-90°C	50-90°C
Current density	0.2-1 A cm^{-2}	0.5-3 A cm^{-2}

Table 2: Summary of the main model parameters.

Variable	Value
Compressor isentropic efficiency	0.8
Electric boiler efficiency	0.98
Discount rate	5%
O&M	2% of the CAPEX
Operating hours	8000 h/y
Electricity price	79.2 €/MWh
Heat price	30.7 €/MWh
Electricity emission factor	0.164 kg/MWh
Heat emission factor	0.244 kg/MWh

RESULTS AND DISCUSSION

Designing for waste-heat utilization

Optimal combined system designs

The performance of combined systems optimized using the different design approaches are shown in Figure 2. The results are consistent with our previous work on atmospheric alkaline electrolyzers only [3]: also for LP and HP PEM electrolyzers, the separate design leads to suboptimal solutions, whereas the combined design allows optimal trade-offs between cost and emissions, depending on the heat output of the system.

In terms of the electrolyzer operating conditions, the combined design leads to more compact electrolyzers with higher current densities, because the additional waste heat can be valorized. Moreover, operating at a higher pressure increases the optimal current density.

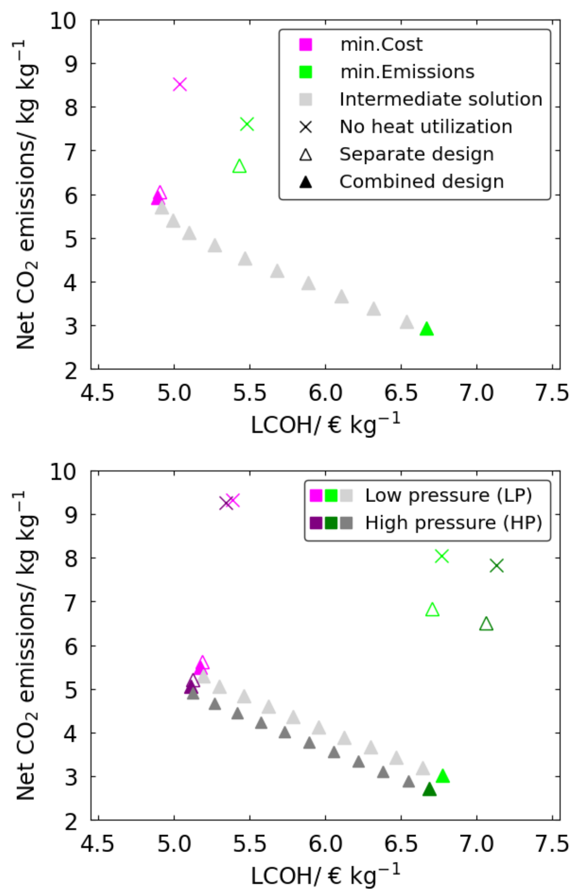

Figure 2. Trade-off between levelized cost of hydrogen (LCOH) and net CO_2 emissions for the combined system with alkaline (top) and PEM (bottom) electrolyzers. Both cost and emissions are given per kg of hydrogen and consider sales revenues and avoided burden, respectively, for the generated heat.

When minimizing costs, the combined systems

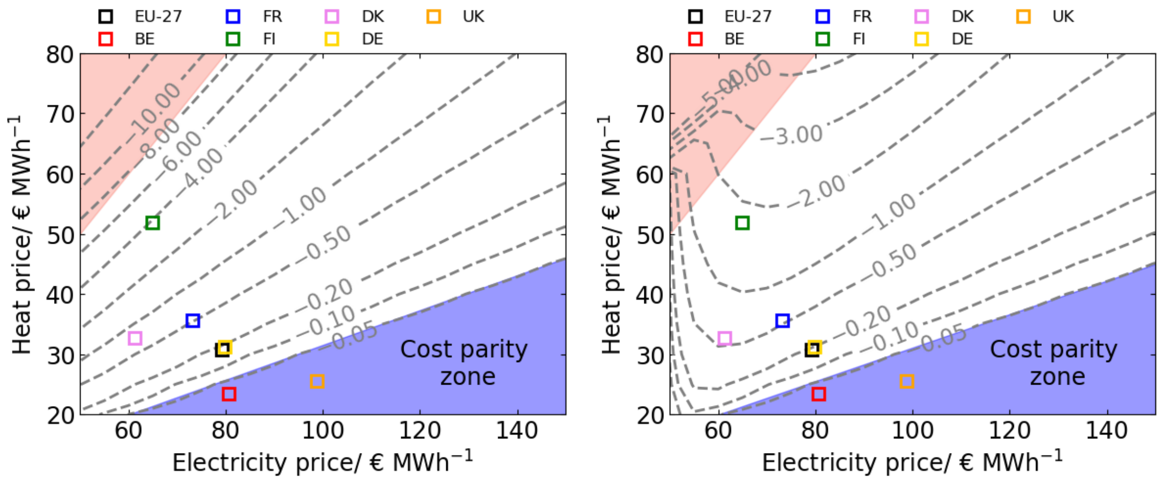

Figure 3. Percentage cost reduction of the combined design over the separate design of the combined system based on alkaline (left) and HP PEM (right) at different energy prices. The blue area indicates the area where both designs have the same cost. The red area indicates an area of unlikely price combinations, in which the heat price is higher than the electricity price. The squares indicate average price in different EU countries in 2016-2020 [9].

based on PEM are more expensive than those based on alkaline, mainly due to their higher CAPEX. Remarkably, HP PEM allows lower cost than LP PEM because (i) the increase in CAPEX due to the pressure factor of 1.2 is offset by an 80% reduction in compression costs (saving nearly 40 M€), and (ii) the higher waste heat available resulting from operation at higher current density is valorized via the heat pumps.

When minimizing emissions, the combined designs allow significant emission reductions but are generally more expensive than the separate designs (filled vs. unfilled green triangles). This is because in the separate designs, the optimizer selects an electrolyzer with the highest efficiency in terms of electricity consumption (highest temperature and lowest current density), significantly reducing the electrolyzer OPEX in exchange of a slight increase in CAPEX. However, for HP PEM, the increase in CAPEX is substantially higher due to the pressure factor, making it more expensive than in the combined design.

Cost benefits over a posteriori coupling

The observed benefit of combined design over separate design holds across various energy price scenarios, especially when electricity prices are low and heat prices are high (see Figure 3). This is evident in the alkaline system, where straight contour lines are observed. However, for PEM systems, curved contour lines appear due to the upper bound on current density.

The higher the current density in the combined design compared to the separate design, the higher the benefit. For alkaline, optimal current densities are typically achieved in the middle of the allowable current density range. In contrast, for PEM, the optimal current densities often reach the upper bound, limiting the system's heat output and, consequently, the heat sales. This limitation is more pronounced in the HP PEM system, where higher current densities are required (Figure 3 right). This suggest that to fully unlock the potential of waste-heat utilization from electrolysis, even higher achievable current densities would be desirable.

Emission benefits over a posteriori coupling

The analysis across various CO_2 emission factors show similar results: The combined design outperforms the separate design, especially at low electricity emission factors and high heat emission factors (up to fourfold reduction). While designing with waste-heat utilization in mind offers limited advantages at low heat emission factors (e.g., heat from biomass), heat is currently still mainly supplied by fossil sources like natural gas. Thus, the combined design remains beneficial in most current scenarios.

Hydrogen and heat supply networks

Optimal supply networks

The cost-optimal hydrogen and heat supply networks to supply a methanol production process and generate steam are depicted in Figure 4. The combined system is the main heat supplier in all the optimal networks, which showcases the potential of the system to contribute to industrial electric heating.

There are no significant differences between the different electrolyzer systems. In all optimal combined systems, the electrolyzer operates at the highest temperature and current density allowed. The slight discrepancy in the amount of heat supplied is due to the different polarization curve (alkaline vs. PEM) and the different

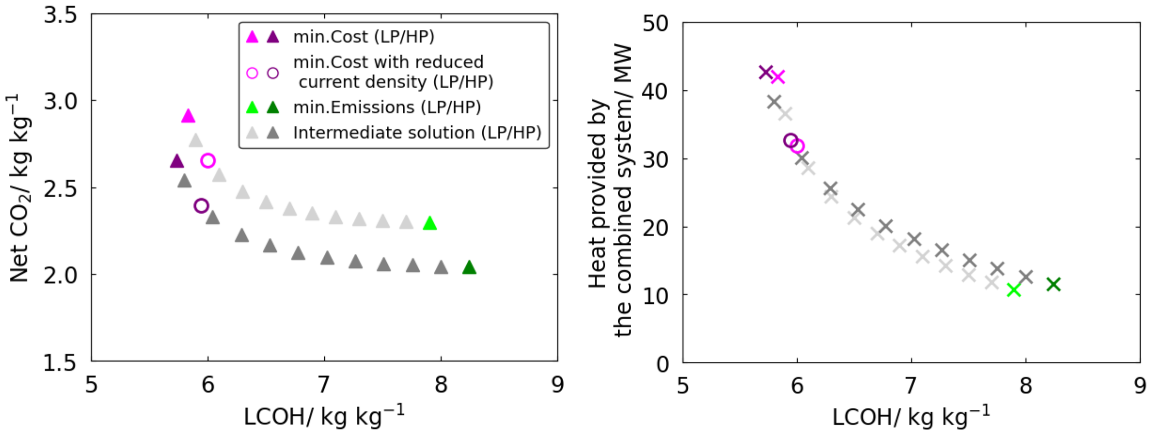

Figure 5. Optimal hydrogen and heat supply networks based on PEM: Pareto front (left) and heat contribution of the combined system in the Pareto-optimal solutions (right).

operating pressure (LP vs. HP).

The air-source heat pump supplies the remaining heat. This technology is preferred over the direct electric boiler for better efficiency and cost advantages from economies of scale.

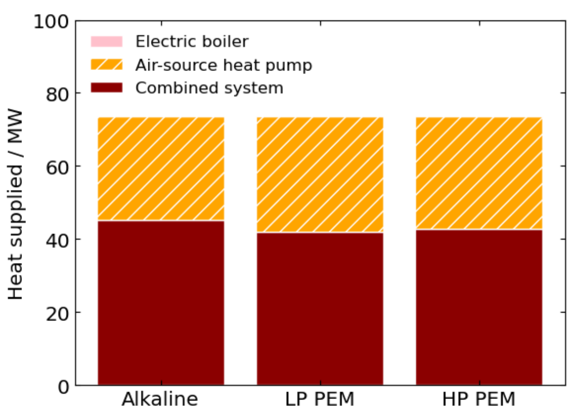

Figure 4. Cost-optimal heat supply networks when using different electrolyzers.

In this work, different heat pumps are considered for each heat source. However, utilizing a heat pump with multiple heat sources (e.g., waste heat, compressor intercooling, and ambient air), could further enhance efficiency, reduce reliance on a single heat source, and increase process reliability. Nonetheless, a cost analysis is necessary to ensure an effective heat supply.

Contribution of the combined system

The cost of the supply network is significantly affected by the amount of heat supplied by the combined system (see Figure 5). While reducing its heat output (i.e., decreasing current density) can lower the net emissions, it also substantially increases costs.

The cost reduction potential compared to the minimum emissions solution depends on the upper bound of the current density. When considering a reduced upper bound of current density (0.7 A/cm2 for alkaline and 2 A/cm2 for PEM), the cost-optimal solutions result in a higher minimum cost (unfilled circles in Figure 5). Therefore, further advances in electrolyzer development to operate at higher current densities are desirable.

Sensitivity analysis

A sensitivity analysis is conducted to assess the impact of electrolyzer investment costs and energy prices (i.e., electricity and heat) on the optimal supply network design and cost. The combined hydrogen and heat supply network is re-optimized for each parameter value.

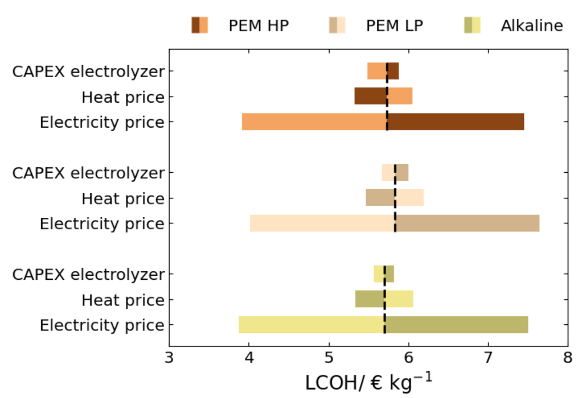

Figure 6. Influence of +30% changes in the electrolyzer CAPEX, heat price and electricity price on the optimal levelized cost of hydrogen.

The optimal combined system design remains unaffected by these parameters, indicating the robustness of the system across a wide range of scenarios. Nonetheless, the resulting cost varies depending on the specific parameter being considered (see Figure 6).

Electricity price has the biggest impact due to the high contribution of OPEX in the cost breakdown. Conversely, investment cost has the lowest influence because of the lower contribution of CAPEX.

The influence of electricity and heat prices is similar across the three electrolyzer systems. However, the investment cost has a greater influence on PEM compared to alkaline systems, as PEM are more expensive.

CONCLUSIONS

The combined system, i.e., electrolyzer with a heat pump, was analyzed for supplying hydrogen to a methanol production process while producing heat suitable for steam production. Waste-heat upgrading from alkaline and PEM electrolyzers offer similar benefits, with the choice depending on the hydrogen needs. Alkaline electrolyzers are cost-effective for large-scale production, while PEM electrolyzers, despite higher upfront costs, provide higher hydrogen purity and flexibility.

Optimizing electrolyzers for both hydrogen and heat production is more beneficial than using the waste heat a posteriori from an electrolyzer optimized solely for hydrogen production. This new approach leads to more compact electrolyzers with higher current densities, reducing costs by up to 10% and CO_2 emissions by four times. Therefore, increasing the maximum achievable current densities can improve waste-heat utilization. The effect of the electrolyzer operating pressure is not significant, as the increase in CAPEX is offset by the reduced compression requirements (about 80% cost reduction).

The combined system is always selected over alternative electric heating technologies in the optimal hydrogen and heat supply networks. Notably, its optimal design remains consistent despite uncertainty in electrolyzer investment cost and energy prices, with electricity price having the biggest impact. Conversely, electrolyzer investment cost has the lowest impact, being higher for PEM than for alkaline.

Further research can investigate the detailed coupling of electrolyzers and heat pumps using flowsheet models. This analysis will help retrofit existing electrolyzer installations and contribute to the optimal waste-heat utilization of future energy systems.

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