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Performance evaluation and comparison of fuel processors integrated with PEM fuel cell based on steam or autothermal reforming and on CO preferential oxidation or selective methanation

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HIGHLIGHTS

- Modeling of different fuel processors integrated with PEM fuel cell stack.
- Steam or autothermal reforming + CO selective methanation or preferential oxidation.
- Reforming of different hydrocarbons: gasoline, light diesel oil, natural gas.
- 5 kW_e net systems comparison via energy efficiency and primary fuel rate consumed.
- Highest net efficiency: steam reformer + CO selective methanation based system.

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ABSTRACT

The performances of four different auxiliary power unit (APU) schemes, based on a 5 kW_e net proton exchange membrane fuel cell (PEM-FC) stack, are evaluated and compared. The fuel processor section of each APU is characterized by a reformer (autothermal ATR or steam SR), a non-isothermal water gas shift (NI-WGS) reactor and a final syngas catalytic clean-up step: the CO preferential oxidation (PROX) reactor or the CO selective methanation (SMET) one. Furthermore, three hydrocarbon fuels, the most commonly found in service stations (gasoline, light diesel oil and natural gas) are considered as primary fuels. The comparison is carried out examining the results obtained by a series of steady-state system simulations in Aspen Plus® of the four different APU schemes by varying the fed fuel. From the calculated data, the performance of CO-PROX is not very different compared to that of the CO-SMET, but the performance of the SR based APUs is higher than the scheme of the ATR based APUs. The most promising APU scheme with respect to an overall performance target is the scheme fed with natural gas and characterized by a fuel processor chain consisting of SR, NI-WGS and CO-SMET reactors. This processing reactors scheme together with the fuel cell section, notwithstanding having practically the same energy efficiency of the scheme with SR, NI-WGS and CO-PROX reactors, ensures a less complex scheme, higher hydrogen concentration in the syngas, lower air mass rate consumption, the absence of nitrogen in the syngas and higher potential power of the stack anode exhaust. The stack anode exhaust, in fact, is recycled to the fuel processor section, thanks to the presence of methane produced in the final clean-up methanation reactor.

1. Introduction

The European Union is committed to transform its economy into a highly energy-efficient, low carbon economy, so it has set targets to reduce greenhouse gas emissions progressively up to 2050. In December 2008 the European Council confirmed a new target to be achieved within 2020: instead of a reduction of 20% of the emission levels of 1990, the new 2008 target was set at a reduction of 30% [1].

A larger use of clean technologies could, in fact, drastically reduce air pollution [2–6], diminishing people diseases and favoring also the global economy [7]. In this way it is expected that the EU could save up to € 88 billion a year by 2050 [1].

Hydrogen-fueled proton exchange membrane fuel cells (PEM-FCs) offer a promising opportunity with the potential to significantly mitigate oil dependency, greenhouse gas emissions and local air pollution [8]. Hydrogen could be considered a superior

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energy carrier, but severe storage and distribution problems still exist. Consequently, its generation via fuel processor units (FPUs) could be a possible short-term intermediate solution [9,10].

The auxiliary power units (APUs) containing FPUs integrated with PEM-FCs provide relatively high efficiency with significantly reduced emissions and low noise generation, compared to the less complex APUs based on internal combustion engines (ICEs) directly fed with diesel oil [8,11,12]. The efficiency of the former APU type remains almost constant even at turn-down operation to less than 50% of full capacity. Moreover, the water produced in the PEM-FC stack can be used in other items of the APU [13]. APUs can be used for mobile applications (trucks, recreational vehicles, and marine leisure), as well for stationary ones (power supply to antennas in remote locations as Uninterruptible Power Supply (UPS) units) [10,13–20].

Particularly in the mobile sector, PEM-FCs are preferred because they are reliable and can be started and stopped very quickly [21]. Instead, for stationary applications, PEM-FC, solid oxide SO-FC or molten carbonate MC-FC can be used, depending on the required power [22–26]. Natural gas (NG), whenever available, is the likely fuel choice [27]. In remote areas where NG infrastructure is still not established, fuels such as propane/LGP and higher liquid hydrocarbons represent competitive alternatives, thus emphasizing the feature of fuel flexibility [27,28].

The development of APUs based on fuel cell with auxiliaries integration and control remains a tricky technical challenge [10,29,30]. This makes it difficult a rational selection of fuel processing reactors for direct hydrogen production [31–34]. Reforming processes, as the steam reforming (SR) or autothermal reforming (ATR) or the partial oxidation (PO) or the oxy-steam reforming (OSR), can be considered viable alternatives [10,14,35–41]. The hydrogen rich gas (syngas) produced this way contains CO, which is a poison for the Pt based electro-catalysts of PEM-FCs. Consequently, the CO concentration in the syngas needs to be lowered down to 10 ppmv prior entering the PEM-FC. The syngas clean-up involves water gas shift (WGS) reactors, reducing CO down to 0.5–1% [37,42,43], and a final CO removal step, feasible by preferential oxidation (PROX) [44–47], or selective methanation (SMET) [48–53], or pressure swing adsorption (PSA) [54,55], or by separation with ionic or metal membranes [56,57], or by electrochemical water gas shift (EWGS) [58,59].

As final clean-up treatment, specific for PEM-FCs, a realistic choice is the CO-PROX or CO-SMET reaction. Both reactions are exothermic and operate at low pressure with the CO selectivity less than 1 and well known pros and cons [60–64]. For PROX selectivity < 1, the complete CO removal is obtained consuming some hydrogen by parallel oxidation, thus making the overall reaction strongly exothermic. The mixing of oxygen (or air) with syngas could be problematic in terms of safety [63,64]. Owing to the SMET selectivity < 1, some CO_2 methanation occurs in parallel. This increases the hydrogen loss, generally in a higher amount compared to CO-PROX [60]. The heat available from CO-SMET is lower (about $^1/_3$) than the one from CO-PROX. For both reactions, the heat available can be recovered [60]. Consequently, the heat of reaction can be integrated. Specifically, in case of CO-SMET, the produced heat can be integrated with the potential heat of the methane produced. Thus, the methane can be more profitably used (from a thermodynamic point of view) by a combustion process somewhere else in the APU system [10]. Last but not least, the CO-SMET reactor is inherently easier to be controlled and regulated [48,49].

In the recent years many research projects and studies were focused on the development of a great number of different types of APU to deliver energy via hydrogen production [8–30]. The scheme differences, mainly concentrated in the fuel processing section, pave the way to compare the performance of at least the base APU schemes to identify the most suitable one.

In the present work the steady-state system simulation technique using Aspen Plus® is employed to examine four base APU schemes to evaluate, and then compare, their global performance. The steady-state system simulation procedure is a very useful tool to evaluate the performance of quite complex systems, like APUs are. This is true especially when the operative conditions and the characteristic working parameters of each item of the system utilized in the model have been experimentally validated. This is the case for the main items considered in the examined APU schemes. Therefore, the preliminary results from the simulations supply unique data, appropriate to proceed with the design and construction of a prototype. From the management of a prototype it is expected either the validation of each single item performance or, above all, the highlighting of possible control and management problems (often arising in systems with a high level of integration as the APUs are), i.e., essential information for the correct design of the final apparatus for the market.

The complexity of a fuel-cell-based APUs is liable of the actual general situation: in the open literature there are not experimental validations of the whole apparatus, but at least of the fuel processing section [14–16,28,30], most of the time realized with heavy governmental grants [61]. Various companies, investing money and resources, are working on the development of reliable APUs to enter the selling markets (see the EU situation in [10], and [30]), but they are slowed down by technical and economic difficulties (in the EU area only one company possesses a marketable apparatus [10]). Moreover, as expected, no detailed technical information are available. Few info are also available from the Japanese/Korean [65–69] and American markets [69–76].

The four APUs investigated in this study consider two of the more commonly employed reforming reactors (steam or autothermal reforming, SR or ATR) for the fuel processing section, and the two final CO clean-up systems of preferential oxidation or selective methanation, CO-PROX or CO-SMET. Each APU scheme contains the SR or ATR reactor and the CO-PROX or CO-SMET reactor, acting as final CO clean-up step of the produced syngas, and in-between a non-isothermal water gas shift (NI-WGS) reactor, common to each scheme. Moreover, a PEM-FC stack provides the power in each APU. The necessary balance of plant (BoP) items are also considered to let each APU operate properly: heat exchanges, afterburner, water injectors, water coolers, water separators, radiators, pumps, and air compressor. An overall APU power of 5 kW_e net is assumed. Typical requirements of the APUs for trucks and passengers vehicles are, in fact, based on the delivery of 5 kW_e net [14,15,77–86].

The main goal of the study is to investigate on the global performance of the four APUs throughout:

- The variation of the energy efficiency and of the consumed primary fuel mass rate. Three of the most widely hydrocarbon feedstocks are considered: light diesel oil (LDO), gasoline (G) and natural gas (NG); their physical–chemical properties are listed in Table 1 [87,88].

Table 1
Physical–chemical properties of the examined primary fuels: natural gas (NG), gasoline (G) and light diesel oil (LDO) [87,88].

	NG	G	LDO
Formula	CH_4	$C_{7.93}H_{14.80}$	$C_{12.32}H_{22.17}$
Molecular weight (kg kmol^{-1})	16	110	170
Hydrogen-to-Carbon molar ratio H_2/C	4	1.87	1.8
Heat of vaporization (kJ kg^{-1})	509	305	270
Liquid specific heat (kJ kg^{-1} K^{-1})	0.63	2.4	2.2
Vapor specific heat (kJ kg^{-1} K^{-1})	2.2	1.7	1.7
Higher heating value HHV (MJ kg^{-1})	55	47.3	44.8
Lower heating value LHV (MJ kg^{-1})	50	44	42.5