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Genuine design of compact natural gas fuel processor for 1-kW_e class residential proton exchange membrane fuel cell systems

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ABSTRACT

A newly designed compact natural gas fuel processor, namely KIER prototype III, for 1-kW_e class residential proton exchange membrane (PEM) fuel cell systems has been developed. The system satisfies the main prerequisites for viable application such as 80% thermal efficiency on the basis of lower heating value at full load as well as CO concentration at PrOx exit less than 10 ppm on a dry basis by integrating internal heat exchange network between heat sources, e.g. burner flame, flue gas and reformed gas from reformer exit, and sinks, e.g. water, feed gas and air. The total system volume including insulation is 13.5 L and also the response time at full load appeared to be less than 50 min. This work mainly describes the design strategies and the effects of independent parameters, e.g. SMR exit temperature and turn-down ratio, upon the response changes (carbon conversion and thermal efficiency). To develop an effective heat exchange network of a fuel processor, a commercial process simulation software package, Aspen Plus, has been used. Based on the simulation results of the conceptual design, a coaxial tubular fuel processor has been developed. Besides, the excellence of the thermally integrated system of the developed fuel processor is verified by comparing its actual operation data with the simulation results.

1. Introduction

Compact natural gas fuel processor to supply hydrogen rich gas for polymer electrolyte membrane fuel cell stack can be regarded as a miniaturized chemical plant whose unit processes consist of desulfurizer (ambient adsorption), catalytic steam reforming, water-gas-shift (WGS) reaction, preferential oxidation (PrOx) and auxiliary components (water pump, compressor, heat exchangers and controls) [1–6]. Also, well established natural gas infrastructure for pipeline supply to household makes it attractive for use as a feedstock for small scale stationary distributed power systems. Main issues for early commercialization of fuel processing technology may be the maximization of thermal efficiency, compact fabrication, low cost and rapid response upon initial start-up and load change [7–9]. This means that the engineering design with heat and system integration is a prerequisite to reduce the number of parts required for the hydrogen production unit as well as to minimize the heat loss to the surroundings. The basic strategies for an efficient and cost effective fuel processor design lie in locating each unit process to induce cascade or spontaneous heat flow from higher to lower temperature and also maximizing internal heat exchange efficiency between heat sources, e.g. flue gas and reformed gas from reformer exit, and sinks, e.g. water, natural gas and air, to optimize thermal efficiency [8–12]. In addition, it is important to maximize the apparent catalytic performance in each unit process by inducing homogenous mixing and uniform distribution of reactants (natural gas and steam) through the entire catalytic bed [13–15].

The main objective of this work is to introduce a highly efficient compact fuel processor designed by KIER for the hydrogen rich gas supply to a 1-kW_e PEM fuel cell cogeneration system with residential use. For this purpose, a design strategy based on process simulation has been applied. In this work, a commercial process simulation software package such as Aspen Plus has been used for designing and optimizing the heat exchange network of a fuel processor. As a reference, some guidelines for fuel processor design are as follows:

1) The natural gas as a feedstock for hydrogen consists of 90% CH_4, 6.63% C_2H_6, 2.25% C_3H_8, and 0.9% C_4H_{10} with 3.8 ppm of sulfur as odorants, where mixing ratio of tetrahydrothiophene/*tert*-butyl mercaptan is equal to 7/3.
2) The thermal or fuel processing efficiency of a viable fuel processor should give greater than 80% as a higher-heating-value (HHV) basis over all load changes.
3) The exit concentration of CO in hydrogen rich gases should be lower than 10 ppm (prerequisite inlet condition for PEM stack).

Based on the developed concept of the heat exchange network in the fuel processor, we have developed a coaxial cylinder-type fuel processor and the excellence and stability of the thermally integrated fuel

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Table 1
Heat sources and sinks in a fuel processor [16].

Reaction zone and temperature	Reaction	Heat source/sink
Burner (900 – 1000 °C)	$C_xH_y + (x + y/4)\ O_2 \rightarrow xCO_2 + y/2\ H_2O$	Source
SMR (600 – 900 °C)	$CH_4 + H_2O \rightarrow CO + 3\ H_2\ \Delta H = 206$ kJ/mol	Sink
WGS (250 – 300 °C)	$CO + H_2O \rightarrow CO_2 + H_2\ \Delta H = -41$ kJ/mol	Source
PrOx (100 – 150 °C)	$CO + 1/2\ O_2 \rightarrow CO_2\ \Delta H = -283$ kJ/mol	Source
Evaporation of water	H_2O (liquid) $\rightarrow H_2O$ (vapor) $\Delta H = 41$ kJ/mol	Sink

processor are verified by comparing the actual operation data with the simulation results.

2. Model-based design of a fuel processor

2.1. Conceptual design of the heat exchange network of a fuel processor

The fuel processor consists of 3 reaction zones and a burner. Since the cost-effective design of the system is directly related to the energy efficiency, the optimal design of the heat exchange network (HEN) is necessary. To design an optimized HEN of a fuel processor, an ordinary analysis on heat sources and sinks in the system should be carried out as the first step. According to the operation temperatures and the reaction heats of the reaction zones in the fuel processor (*see* Table 1), the heat sources are obviously a burner, hot reformates, exothermic WGS reaction and PrOx zones. Meanwhile, the major heat sinks are a catalytic steam-methane reforming (SMR) zone and a preheater for the feed stream including both fuel gas and water.

Based on the analysis for heat sources and sinks, we have carried out basic calculation for defining the net heat duty and the theoretical maximum energy efficiency of the 1-kW_e fuel processor. The relevant assumptions for the calculation are as follows:

- Heat exchanger efficiency is assumed to be 100%.
- For 1-kW_e fuel processor, the flow rate of the methane feed is 12 mol/h and the steam-to-carbon molar ratio (S/C) is set to be 3.
- The temperature of feed gas is 20 °C and the temperature of the product gas fed into the fuel cells is 90 °C.
- The overall energy efficiency of the fuel processor based on lower heating values (LHVs) is calculated by Eq. (1) assuming that the feed gas is pure methane.

$$\eta(\%) = \frac{H_2 \text{ production rate} \times \text{LHV of } H_2}{\text{net heat duty} + \text{flow rate of } CH_4 \times \text{LHV of } CH_4} \times 100 \qquad (1)$$

where LHV of H_2 and CH_4 is 244 kJ/mol and 802 kJ/mol, respectively.

- The calculation is carried out by Aspen Plus, commercial process simulation software, where the Peng–Robinson equation of state is chosen as a physical property method and the equilibrium reactors (REquil) are used [17].

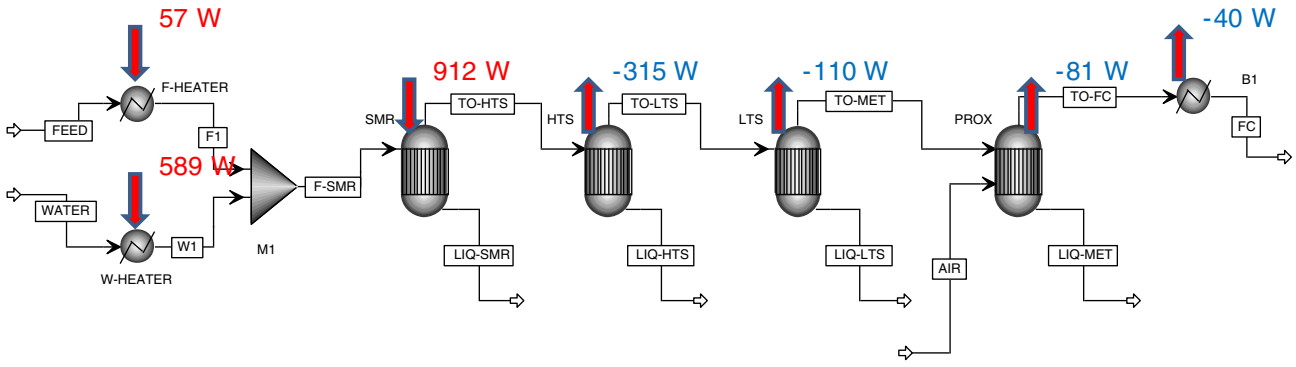

Fig. 1. Analysis on heat duty of each unit in a fuel processor.

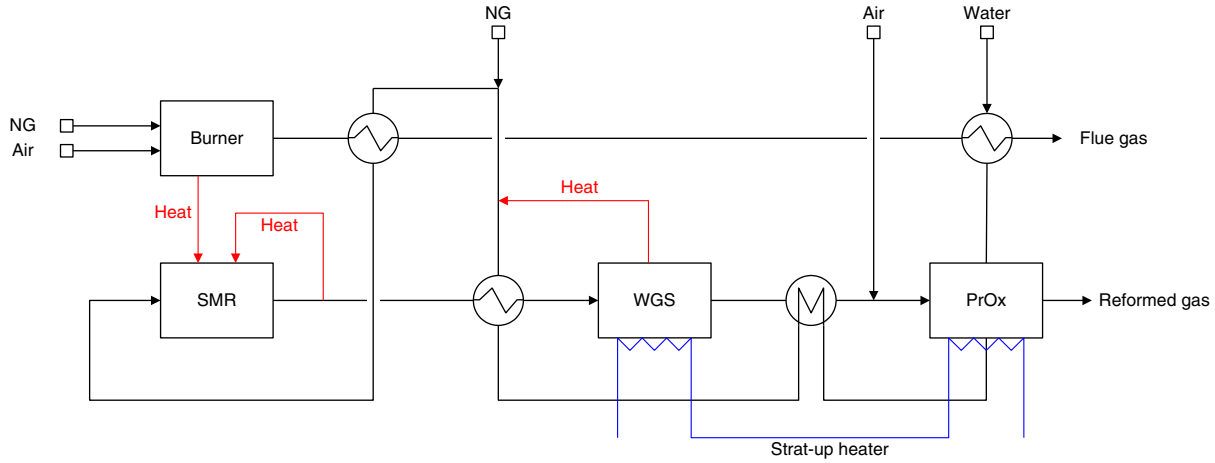

Fig. 2. Conceptual design of the overall heat exchange network of the fuel processor having a burner.