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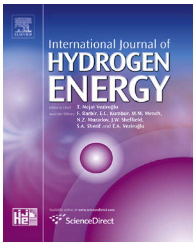

A process simulation study of a newly designed fuel processing system for a high temperature PEM fuel cell unit

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ABSTRACT

Fuel cells can be one of the ideal technologies for micro-cogeneration and also for Uninterruptible Power Supply systems (UPS) especially in terms of high reliability, low environmental impact and size flexibility. A micro-cogeneration system provides electricity and heat whereas UPS system provides electricity during a shortcut. Since those units have capacities of 1–5 kWe, they are developed for residential applications. Both UPS and micro-chp units for high temperature PEM fuel cell should contain a fuel processor which converts natural gas, LPG or other hydrocarbons into hydrogen rich (up to 50%molar) synthesis gases via reforming and water-gas shift reactions. These units also contain an afterburner fueled by PEM anode off-gas to provide preheating of inlet streams of hydrogen production reactor.

In this work, a newly designed “micro scale compact fuel processing system” for hydrogen rich gas production to be used for a 1 kW_e High Temperature Fuel Cell (HTPEM) is presented and thermodynamically analyzed. Natural gas has been simulated as a hydrocarbon fuel source in the flow-sheet model. The overall fuel processing system is simulated using ASPEN HYSYS process simulation package. The simulated fuel processing system (FPS) has been integrated with a high temperature PEM fuel cell unit. FPS has been modeled to determine the thermodynamic characteristics of the overall process. The steady-state simulations have been realized for the overall process. The changes on reactor temperatures, feed flow rates, steam to carbon ratios, compositions and electrical loads have been investigated.

Introduction

Fuel cell based systems have received increasing attention recently due to their significant advantages. First of all, fuel cell based systems are considered especially for the local electricity generation hence they are convenient in distributed power grid structure which minimizes transmission losses of electricity. Secondly, a well-developed infrastructure for distributed natural gas is already presented in several countries. Therefore, generation of electricity in domestic households started to be vitalized via small-scale energy conversion

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devices such as stirling engines, micro-turbines and fuel cells, micro & small-scale applications from 1 kW_e up to tens of kW_es [1]. Among fuel cells, a range of different types exists including proton exchange membrane (PEM) and solid oxide fuel cells (SOFC) [2].

Stationary fuel cell based power generation systems offer a great market opportunity, because the technology is capable of achieving higher reliability, higher efficiencies, higher flexibility in size with lower emissions as compared to conventional power systems [3].

A micro-CHP system provides electricity and heat (space heating and hot water) for a residential building demand. These systems are designed to convert the chemical energy in a hydrocarbon feedstock into both electrical power and useful heat [4].

In the last decade, micro-CHP based on PEM fuel cells has been intensively developed. Most of these systems are based on low temperature PEM fuel cells which operate at less than 100 °C. Several studies about PEMFC based CHP processes can be found in open literature. Recent progress has focused to develop PEM fuel cells that operate above 100 °C. There are several reasons for operating at a higher temperature: (i) Electrochemical kinetics for both electrode reactions are enhanced; (ii) Water management can be simplified because only a single phase of water need to be considered; (iii) The cooling system is simplified due to the increased temperature gradient between the fuel cell stack and the coolant; (iv) Waste heat can be recovered as a practical energy source; (v) CO tolerance is dramatically increased thereby allowing fuel cells to use lower quality reformed hydrogen [5].

As a result of these improvements, simplified purification processes in reformers are required. Polybenzimidazole (PBI) based fuel cells are normally referred as High Temperature Proton Exchange Membrane Fuel Cells (HTPEM) in contrast with Nafion based Low Temperature Proton Exchange Membrane (LTPEM) fuel cells which require high purity hydrogen. The electrochemical kinetics of the reactions of the HTPEM fuel cells are improved via the higher temperature range of 160°C–200 °C by using PBI based membranes [6,7].

Although attention to HTPEM fuel cells has been growing, most research activities concern with membrane modeling or experimental characterization of stacks and only few with CHP systems [8]. The prototypes exist based on reforming of natural gas and high temperature proton exchange membrane fuel cells (HTPEMFC).

Currently the fuel cell technology based on hydrogen rich reformate gas has made the market penetration. For instance, the Ene-Farm project, presented by Tokyo Gas that represents 35% of the Japanese gas market in Japan, subsidized the introduction of cost competitive 1 kW fuel cell systems operated on reformate gas and reached the 100.000 system installations in 2014. Propane, natural gas as well as liquid hydrocarbons are currently the preferred fuels because of their high storage density for hydrogen generation in fuel cell applications. Using these fuels the existing infrastructure can be used until hydrogen becomes widely available.

Recently, high temperature PEM fuel cells have more attention to find new alternative power production routes. These type of fuel cells are also one of the most promising technology for several areas, such as stand-alone power units [9], auxiliary power, Combined-Heat-and-Power (CHP), portable generators and remote applications [10–13].

Fuel cells working at temperatures below 100 °C (common PEM technology) can only be operated with CO contents that are lower than 100 ppm [14]. Therefore hydrogen purification reactors, especially preferential oxidation steps, are necessary in order to reduce CO content to ppm level. The high temperature PEM fuel cell can tolerate CO contents of up to 3% vol. at operation temperatures around 180 °C [15]. After reforming of hydrocarbon fuels, this required CO level within water-gas shift reactors without further any preferential oxidation steps. Hence HTPEM systems are simpler. Fuel cells working at very high temperatures that is 750 °C and higher (e.g. SOFC) don't need any hydrogen rich gas clean-up steps after the reforming process. The system is much simpler but those fuel cells are not suitable to use in applications where quick start-ups or dynamic operation modes are required since they usually have problems of thermal stress of the materials and sealing.

It is acknowledged that the fuel processing systems can have a major affect for the overall fuel cell system efficiencies, process unit costs and common practices [16–19]. Fuel processing and/or reforming systems are being widely developed to be used for on-board and stationary applications [20,21,6].

In this study, a newly designed “micro scale compact fuel processing system” for hydrogen rich gas production for a 1 kW_e High Temperature Fuel Cell (HTPEM) is presented and thermodynamically analyzed. The fuel processing system consists of auto thermal reformer (ATR) and high & low temperature shift reactors (HTS, LTS). The effects of operation parameters on the product gas content and on the efficiencies are discussed in details.

Methodology

The ASPEN HYSYS v8.4 process simulation software has been used for the calculations of the whole integrated process, i.e fuel processing system and fuel cell. Natural gas has been simulated as a hydrocarbon fuel source in the flow-sheet model. The chemical composition of the natural gas is 95.22% methane, 3.22% ethane, 0.79% propane; and balance i-butane, n-butane and nitrogen. The average molecular weight and mass density of natural gas feed is about 16.87 kg/kmol and 0.69 kg/m^3.

HTPEM fuel cell operates with hydrogen-rich gas at maximum acceptable CO concentration limit of 1.5%. Parametric process simulation studies have been conducted to find the compositions, efficiencies and load profiles. The effects of the inlet temperature of ATR reactor, the steam to carbon (S/C) and oxygen to carbon (O_2/C) ratios (Eqs. (1) and (2)) have been investigated. Steam/carbon ratio is especially critical in terms of avoiding carbon deposition on the catalyst and the realization of endothermic steam reformer reactions. Oxygen/carbon ratio has also critical importance in the progression of the exothermic partial oxidation reactions. The efficiency of hydrogen production reduces if this rate is high. At the same time higher O_2/C ratios also cause an increase of the reactor temperature.