

Model-based investigation of a CO preferential oxidation reactor for polymer electrolyte fuel cell systems

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Abstract

This paper deals with a two-dimensional model of a preferential oxidation (PROX) reactor to be used in a beta 5 kWe hydrogen generator, named HYGen II, to integrate with polymer electrolyte fuel cells (PEFCs) for residential applications. The reactor geometrical configuration developed is a single-stage multi-tube configuration, in which a cocurrent air flow in the interspace is aimed at improving heat transfer and consequently controlling the temperature of the reactor. The aim of the model is to investigate the process performance of the reactor in order to enhance optimization and control of the PROX unit. The model concerns chemical kinetics and heat and mass transfer phenomena in the reactor. The model plays a key role in overcoming the issues of system design, by evaluating the temperature and the gas concentration profiles in the reactor. The CO removal from simulated reformat was examined with varying inlet temperature. Simulation results showed the strong dependence of the overall performance upon the reactor geometrical configuration.

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1. Introduction

During the last few years fuel cells have been considered to be promising tools for energy conversion from both industrial R&D departments and academia. The polymer electrolyte fuel cell (PEFC) fuelled by hydrogen appears to be the key option for both transport and small scale combined heat and power applications, due to its compactness, modularity, higher conversion efficiencies and low emissions of noise and pollutants [1,2]. A growing interest for small stationary applications (in the 0.5–10 kW electrical output range) is developing, with a large increase in the number of installed units in the world, as a decentralized power supply, grid support, peak shaving, power back-up or uninterruptible power supply (UPS), can be derived [3].

The absence of a hydrogen refuelling infrastructure and problems concerning hydrogen storage, has led to the development of fuel processors able to convert available fuels (hydrocarbons and/or alcohols) into hydrogen rich reformat gas [4].

The choice of a suitable fuel processor and fuel, during the transition phase to a hydrogen economy, are key aspects to the successful implementation of direct-hydrogen fuel cell systems.

The key requirements for a fuel processor include rapid start-up, good dynamic-response to change in hydrogen demand, high fuel-conversion, small size and weight, simple design (construction and operation), stable performance for repeated start-up and shut-down cycles, maximum thermal integration, low cost and maintenance, high reliability and safety [5].

In small scale applications, natural gas remains the fuel most commonly employed for its wide availability and related infrastructure. For some niche markets, such as electricity production in remote sites, LPG could be an interesting optional fuel [6,7]. However, to utilize the reformat gas as a reactant for PEFC systems, clean-up steps must be considered to reduce the CO concentration to an acceptable level (10 ppm), since the fuel cell performance is progressively degraded by CO poisoning of the anode catalyst [8,9]. The reformat stream is purified using a two-stage process. The first stage is the water gas shift reaction, that reduces the carbon monoxide, increasing hydrogen content. The CO conversion is limited by equilibrium at the outlet temperature of the reactor. In the second stage the amount of

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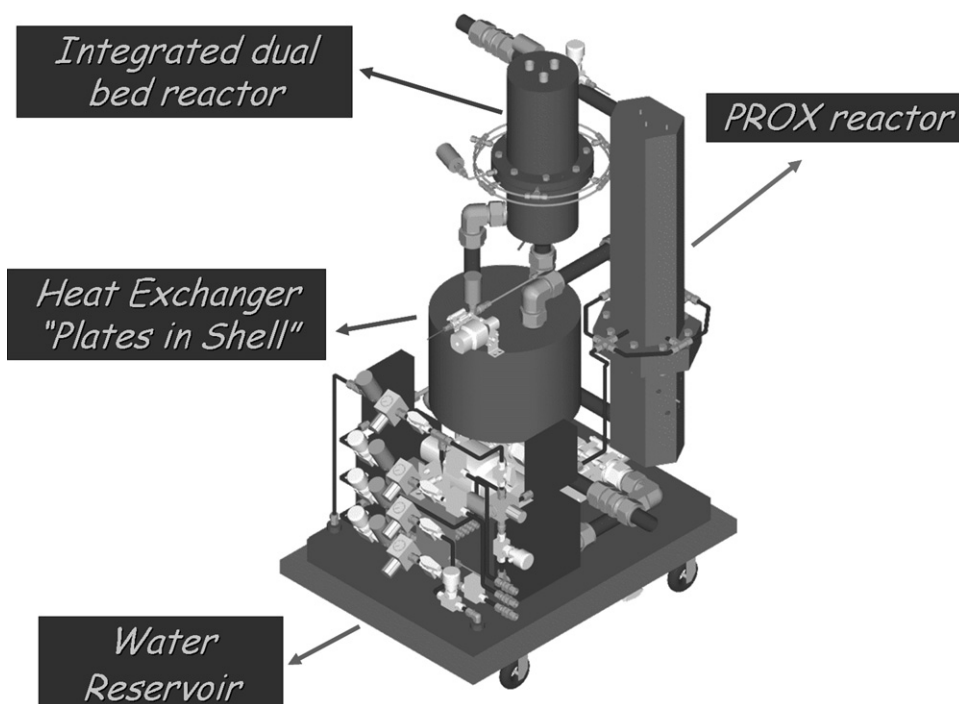


Fig. 1. Diagram of the 5kWe hydrogen generator (HYGen II).

carbon monoxide is further reduced using preferential oxidation, that is the most compact of all the purification methods. Alternative technologies for the last clean-up step, such as pressure swing adsorption (PSA) or metal separation membranes, are not suitable for small scale applications, because high pressure requirements mandate the use of an additional compressor, and the need to re-humidify the hydrogen prior to use in fuel cells. Furthermore, a desiccant must be used to adsorb water from the incoming wet gas stream in a PSA unit [10].

Because the PROX reaction is exothermic, the main drawback of a preferential oxidation reactor is that it requires complex temperature control systems, in order to minimize parasitic hydrogen oxidation, since selectivity of oxygen to carbon monoxide deteriorates with increasing operating temperatures [11]. The consequent oxidation of hydrogen causes a decrease in the process efficiency and increases water management issues. Multi-stage PROX reactors have been proposed [12–14], but complex hardware is required to control temperatures, using staged air injections along the catalyst bed. A single-stage PROX process could be an optimal solution, as reported by Echigo et al. [15]. It has been reported that Ru/Al₂O₃ catalysts showed higher CO removal performance than conventional Pt/Al₂O₃ catalysts [16–18].

During the last few years, research activity on the PROX reaction for small scale applications has focused on catalyst development and testing and reactor design optimization, in order to reduce the CO concentration to below 10 ppm to meet the fuel purity requirements for PEFC stacks.

Previous experimental tests with our 2kWe LPG based fuel processor (HYGen I) [19], designed for integration with a PEFC, showed some drawbacks in the CO preferential

oxidation step: the CO content in the output of the reactor reached a CO level of 0.2% (dry basis). This content, incompatible with PEFC, showed the need of improving the prototype engineering, focusing on further efforts to achieve optimized design of the PROX subsystem, in terms of temperature control.

The objective of this study is to theoretically investigate the PROX kinetics by a modeling approach. A two-dimensional steady state reactor model was developed, driving the design of a single-stage multi-tube reactor to overcome the system issues of heat management. This geometrical configuration, with a cocurrent air in the cooling jacket (interspace), is used as a case study in developing a beta 5kWe hydrogen generator [20,21]. The results of the simulation were compared with other two geometrical configurations: without a cooling jacket and with a countercurrent air flow in the interspace. The simulation studies make it possible to gain insight into the factors that limit PROX performance.

2. Design approach

The HYGen II system can generate hydrogen for PEFCs for small stationary applications. The prototype is able to convert light hydrocarbons (methane, propane, LPG, butane) with a nominal hydrogen production of 5 Nm³ h⁻¹ and a maximum hydrogen production of 8 Nm³ h⁻¹. The net size (mm) of the fuel processor is 636 (width) × 868 (length) × 1350 (height).

The unit is based on three catalytic reaction steps: the auto-thermal reforming (ATR), the intermediate water gas shift (ITWS) and the preferential oxidation (PROX). The diagram of the integrated system is shown in Fig. 1; the processing unit is coupled with a heat exchanger, a static mixer,

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