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Design and control of energy integrated SOFC systems for *in situ* hydrogen production and power generation

Dimitrios Georgis[a], Sujit S. Jogwar[a], Ali S. Almansoori[b], Prodromos Daoutidis[a,*]

[a] Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, USA
[b] Department of Chemical Engineering, The Petroleum Institute, Abu Dhabi, United Arab Emirates

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ABSTRACT

This paper studies the design and operation of energy integrated solid oxide fuel cell (SOFC) systems for *in situ* hydrogen production and power generation. Two configurations are considered: one where the hot effluent stream from the fuel cell is used directly to provide heat to the endothermic reforming reaction, and another where the hot effluent streams are mixed and combusted in a catalytic burner before the energy integration. A comparative evaluation of the two configurations is presented in terms of their design, open-loop dynamics and their operation under linear multi-loop controllers.

1. Introduction

Fuel cells provide the most efficient path for the conversion of chemical energy into electrical energy (Varigonda & Kamat, 2006). Recognizing the need for efficient energy production systems and the fact that fuel cells are not limited by Carnot efficiencies, there has been an increasing interest in developing fuel cell systems for stationary and transportation applications (see e.g. Bavarian, Soroush, Kevrekidis, & Benziger, 2010; Bhattacharyya & Rengaswamy, 2009; Chaisantikulwat, Diaz-Goano, & Meadows, 2008; Cresswell & Metcalfe, 2006; Kee, Zhu, Sukeshini, & Jackson, 2008; Pukrushpan, Stefanopoulou, & Peng, 2004; Varigonda & Kamat, 2006, for excellent overviews on recent developments and opportunities in modeling and control of fuel cell systems). Hydrogen is the most preferred fuel for a fuel cell. Given the safety issues associated with the storage and transportation of hydrogen, *in situ* production of hydrogen from a hydrocarbon fuel, coupled with a H_2-fed SOFC, presents a promising approach for power production, especially for stationary fuel cell applications.

Two approaches have been proposed to this end. One of the approaches uses an *external* reformer (e.g. Adams, Thomas, & Barton, 2010; Braun, Klein, & Reindl, 2006; Mueller, Jabbari, Gaynor, & Brouwer, 2007; Murshed, Huang, & Nandakumar, 2007) to generate a hydrogen-rich stream which is then fed to the fuel cell. The other approach uses the principle of *internal* reforming (e.g. Al-Qattan & Chmielewski, 2004; Braun et al., 2006), wherein both the reforming and the electrochemical reactions take place in a single unit. The internal reforming approach offers benefits in terms of energy consumption, however at the cost of operating challenges (carbon deposition on electrodes, fewer inputs available for control, etc.). One variant of this approach uses *indirect internal* reforming, wherein the reforming and the electrochemical compartments are only in thermal contact, thereby avoiding the direct physical contact (Aguiar, Chadwick, & Kershenbaum, 2002). In this paper, we focus on the approach based on external reforming as it offers more opportunities for integration and control design.

A power system consisting of an external reformer and a fuel cell shows a lower overall efficiency, since additional energy is required to drive the endothermic reforming reactions. SOFCs are high temperature fuel cells with an operating temperature range between 800 °C and 1000 °C. The hot stream leaving the SOFC shows potential for energy integration by supplying energy to the endothermic reformer, and thereby improving the overall efficiency. Different integration strategies for SOFC energy systems have been proposed (see e.g. Zhang et al., 2010 which reviews most of these strategies). These include hybrid integration strategies with direct thermal coupling (Chan, Ho, & Tian, 2002; Zhang, Li, Li, & Feng, 2006), indirect thermal coupling (Calė, Santarelli, & Leone, 2006) as well as fuel coupling (Yi, Rao, Brouwer, & Samuelsen, 2005), and advanced integration strategies using gas/humid air/steam turbines (Kandepu et al., 2007; Mueller et al., 2008; Oh & Sun, 2010; Varbanov & Klemes, 2008). Some of these strategies directly (without mixing the anodic and cathodic streams) use the hot SOFC effluent for energy recovery (e.g. Bents, 1987; Sadhukhan,

* Corresponding author. Tel.: +1 612 625 8818; fax: +1 612 626 7246.
E-mail address: daout001@umn.edu (P. Daoutidis).

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Nomenclature

Capital letters

R	Universal gas constant
T	Temperature
F	Faraday constant
V_{FC}	Voltage of single cell
I_o	Exchange apparent current
I	Current
R_i	Resistance of each compartment
I_L	Limiting current
N	Number of cells in the SOFC stack
V	Output voltage
P	Output power
Cp_i	Heat capacity of component
V_i	Volume of each compartment
P_i	Operating pressure of each process
ΔH_i^{rxn}	Heat of reaction
$\dot{Q}_i$	Enthalpy flow
U	Overall heat transfer coefficient
A	Area
ΔT_{LM}	Logarithmic mean temperature difference
U_F	Fuel utilization
L	Length
W	Width

Small letters

n	Number of transferred electrons
p_i	Partial pressure of each species
$\dot{n}_i$	Molar flow rate
m	Mass
r_i	Reaction rate
τ	Thickness

Greek letters

η	Number of transferred electrons
α	Charge transfer coefficient
ρ	Density
ε	Void fraction

Subscripts

FC	Fuel cell
OCV	Open-circuit voltage
act	Activation
ohm	Ohmic
conc	Concentration
an	Anode
el	Electrolyte
ca	Cathode
int	Interconnect
fuel	Fuel stream
air	Air stream
SR	Steam reformer
cat	Catalyst

Zhao, Leach, Brandon, & Shah, 2010), while others use a catalytic burner to further recover energy from the unreacted fuel and use this stream for energy integration (e.g. Chan et al., 2002; Mueller et al., 2007). While each of these approaches has obvious advantages/disadvantages in terms of capital and operating costs, compatibility with downstream processes, and environmental impact, they also offer different opportunities and challenges in terms of overall integrated system design, dynamics and control. This is a rather untouched subject in the literature. Motivated by this, in this paper we compare (and contrast) these two approaches at the design and operational stages. The results of this study can guide the selection of a particular approach. To this end, we consider a generic SOFC energy system with an external methane steam reformer. Energy recovery is achieved by designing a network of heat exchangers (HE). Through open-loop simulations under imposed step changes in the current, the dynamic behavior of each of the configurations is analyzed. Linear multi-loop control strategies are proposed for each case and their operational characteristics are compared through closed-loop simulations.

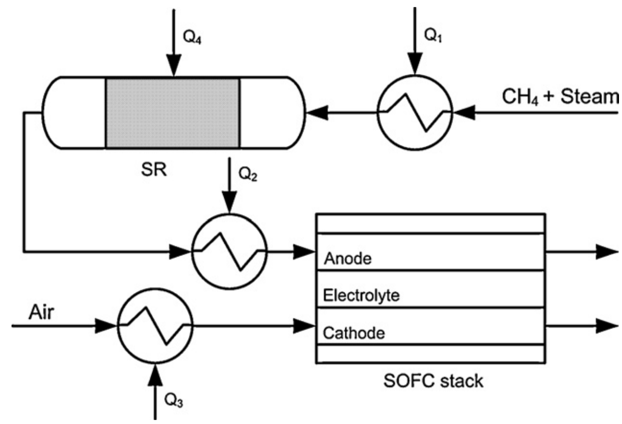

Fig. 1. Generic design structure of the SOFC energy system.

The rest of the paper is organized as follows. The modeling details for the fuel cell and the reformer are presented in Section 2. The selection of operating points for each of these units based on steady state analysis is presented in Section 3. The design, dynamics and control aspects of the energy integrated configurations are analyzed in Sections 4, 5 and 6, respectively. Lastly, Section 7 includes a detailed discussion comparing the two configurations.

2. SOFC energy system with external reformer

A generic SOFC energy system with an external methane steam reformer is shown in Fig. 1. As the reformer and the fuel cell operate at a high temperature, three heat transfer units are required to heat the methane steam mixture, fuel cell anode and cathode inlet streams. Furthermore, energy is required for sustained hydrogen production in the endothermic steam reformer. In the following subsections, we present the modeling details for the fuel cell and the reformer which are the main units of the system.

2.1. Solid oxide fuel cell

The SOFC stack consists of individual cells connected in series. This is a common approach to scale-up the output voltage, thereby resulting in an increased supply of power (NETL, 2004). A hydrogen-rich stream is fed to the anodic compartment of the fuel cell, while air is supplied to the cathodic compartment. The following exothermic redox reactions take place in the fuel cell, thereby generating an electrochemical potential:

$$\text{Anode:}\quad H_2 + O^{2-} \rightarrow H_2O + 2e^-$$
$$\text{Cathode:}\quad \frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}, \qquad \Delta H^{\circ}_{298} = -241.83\,\text{kJ/mol}$$

The open-circuit voltage that can be generated by the fuel cell is given by the Nernst equation:

$$E_{OCV} = E_o(T_{FC}) + \frac{RT_{FC}}{2F}\ln\left(\frac{p_{FC,H_2}\cdot p^{0.5}_{FC,O_2}}{p_{FC,H_2O}}\right) \qquad (1)$$