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# An Energy Integrated Solid Oxide Fuel Cell System: Modeling and Simulation

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**Abstract.** As a solid oxide fuel cell (SOFC) system is under dynamic development for a profitable use in the future, it is very important to understand its transient characteristics. In this paper, the modeling and simulation of an energy integrated SOFC system has been performed to analyze the dynamic characteristics of the heat integration. The lumped models of the energy integrated SOFC system are developed and simulated to present the results of open loop response of the temperatures of SOFC, steam reformer and air inlet stream. The simulation results showed that the air flowrate has a dominant effect on the temperature of SOFC while the valve position and the heater power supply noticeably affect the reformer temperature and air inlet temperature, respectively. Therefore, the match of major influence of input step change on the temperatures of SOFC, steam reformer and air inlet stream in the energy integrated system is very practical for an effective control strategy in the development of control system design.

## Introduction

Due to severe problems of global warming, high pollution, increased demand of energy, and energy security, alternative energy sources are urgently needed. It has been known that fuel cells have attracted extensive interest as highly effective and environmentally acceptable systems because they can convert chemical energy to electrical energy and heat directly from fuels through electro-chemical reactions at electrodes. Among different fuel cell technologies, a solid oxide fuel cell (SOFC) can offer the widest potential range of applications and high system efficiency [1]. The SOFC is remarkably interesting owing to its very high operating temperature range between 1073 and 1273 K at which the hydrogen fuel produced by a steam reformer can be directly fed into the anode side of SOFC since SOFC cannot be poisoned by carbon monoxide that makes it highly fuel-flexible. The *in situ* hydrogen production from a hydrocarbon fuel, coupled with hydrogen rich stream fed to the SOFC presents a promising approach for power generation, especially for stationary fuel cell applications [2]. Among renewable sources, ethanol is a promising candidate because it is non-toxic and easily produced by the fermentation of biomass or agricultural waste products. The mixture of hydrogen, carbon dioxide, carbon monoxide and methane is a main product from ethanol steam reforming process.

A SOFC power plant composed of a steam reformer and a fuel cell generally demonstrates a lower overall efficiency because the additional energy is required to force the endothermic reforming reactions. To increase the SOFC overall system efficiency, an energy integration is achieved by designing a heat exchanger network. Various diverse integration strategies for SOFC energy systems have superbly proposed by Zhang et al. [3]. There has been an increasing interest in developing SOFC systems for both stationary and transportation applications and the overall system design, dynamic modeling and process control design are very necessary. In previous work on dynamic modeling of SOFC systems, most interest has been focused on modeling in electrodes, flow channels, SOFC temperature of both planar and tubular stacks as summarized by Huang et al. [4] and a lot of researches have been conducted on the modeling and control of SOFC systems fueled by methane

[5-9]. For the energy integrated SOFC systems, Georgis et al. [2,5] presented the design and operation of an energy integrated SOFC system with an external methane steam reformer. Das et al. [6] performed a model-based analysis of a SOFC system with an integrated steam reformer and with methane as a fuel in order to analyze the steady-state and transient characteristics of the integrated system. There has been some work on the modeling and control of ethanol stream reformer [10] but no report on the modeling and simulation of the energy integrated SOFC system with an ethanol steam reformer. Based on the principle of mass and energy balances, previous numerous papers investigated on the SOFC modeling can be applied for this work.

In this paper, the modeling and simulation of a SOFC energy system integrated with a steam reformer has been carried out. Ethanol is considered as a hydrocarbon-derived resource reformed to be the hydrogen rich gas for the SOFC fuel. The mathematical models of energy balances are extended and simulated to report the results of open loop response of the temperatures of SOFC, steam reformer and air inlet stream. The open loop response is analyzed for the future work of system and control design.

## Overview of an integrated SOFC System

A configuration design of an integrated solid oxide fuel cell (SOFC) system is demonstrated in Fig. 1. The ethanol fuel mixed with water is preheated and then reacted in a steam reformer at which the high energy for the endothermic reaction is required. The hydrogen-rich gas is produced in the reformer and then fed into the anode side of SOFC. Air is preheated before entering the cathode side. The excess air is added to be the extra air supply to keep the SOFC operating temperature as the adiabatic process. Inside the fuel cell, SOFC reactions that take place at anode and cathode to generate both of the electricity and heat can be described as:

$$\begin{aligned}
\text{Anode:}\quad & H_2 + O^{2-} \rightarrow H_2O + 2e^- \\
& CO + O^{2-} \rightarrow CO_2 + 2e^- \\
& CH_4 + 4O^{2-} \rightarrow 2H_2O + CO_2 + 8e^- \\
\text{Cathode:}\quad & O_2(g) + 4e^- \rightarrow 2O^{2-}
\end{aligned} \tag{1}$$

As shown in Fig. 1, there is one hot stream leaving a SOFC unit that the anode exhaust and the cathode exhaust are already mixed. Due to the very high temperature of SOFC and the high amount of excess air, the residual hydrogen and carbon monoxide can be entirely combusted in the mixer without any additional heat and air supply. A small amount of residual hydrogen and carbon monoxide is assumed so the change of temperature after mixing can be neglected. The outlet stream of SOFC unit is recycled through the heat exchanger network to supply energy to the integrated SOFC system. The hot stream from the SOFC unit is split into two streams (hot stream *a* and hot stream *b*). The calculated hot stream *a* must be enough to supply heat for both the steam reformer considered as a heat exchanger (HX1) and the fuel preheater (HX2). The high temperature exhaust of the remaining split hot stream *b* can be used to produce the additional electricity using gas turbine or produce hot steam for industrial use. As the high quality of the high temperature steam production is feasible, the hot stream *b* is initially fed into a heat recovery unit. The hot exhaust stream leaving the heat recovery unit is then supplied for the air heat exchanger (HX3). Although the energy integration is presented that the usable heat of SOFC hot stream is enough for all heat exchangers in the system and for heat recovery to produce the extra electricity, the additional heater for heating air inlet stream before entering the SOFC is designed as a hot utility when the temperature deviation of heat recovery outlet stream appears.

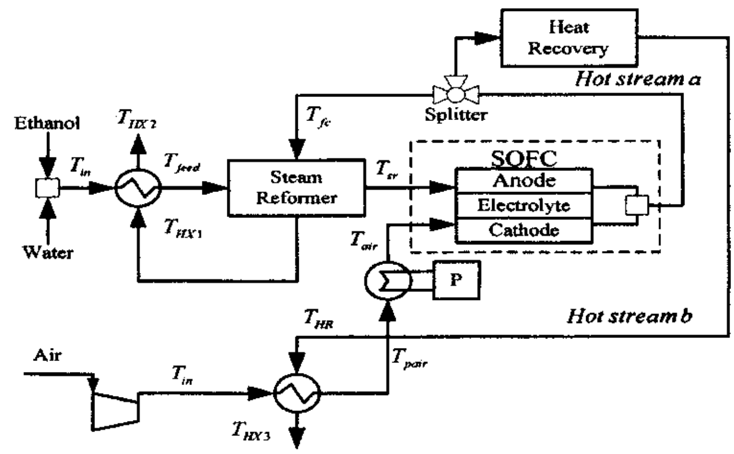


Fig. 1. Basic configuration design of the energy integrated SOFC system.

## Integrated SOFC System Models

Because of the complex mathematical models taking place in the SOFC system, a number of simplifying assumptions are made and described as:

1. All the physical properties are assumed to be uniform over the SOFC, resulting in a lumped model.
2. All the gases are assumed to be ideal.
3. All the gases inside the SOFC stack are perfectly mixed so that the exhaust temperatures of the residual fuel and air from anode and cathode, respectively, are same as the operating temperature.
4. Inlet streams of fuel and air entering the SOFC stack are uniformly distributed to each individual cell.
5. For the energy balances, the changes of pressure within the SOFC are neglected.
6. An adiabatic operation of the fuel cell is assumed.

The lumped models of SOFC stack for the species balance (Eq. 2 – Eq. 4) and the energy balance (Eq. 5) can be given as

$$\frac{dN_{H_2,fc}}{dt} = \dot{N}_{H_2,f} - \dot{N}_{H_2,fc} - \frac{I}{2F} \tag{2}$$

$$\frac{dN_{O_2,fc}}{dt} = 0.21\dot{N}_{air} - \dot{N}_{O_2,fc} - \frac{I}{4F} \tag{3}$$

$$\frac{dN_{H_2O,fc}}{dt} = \dot{N}_{H_2O,f} - \dot{N}_{H_2O,fc} + \frac{I}{2F} \tag{4}$$

$$\rho_{fc}V_{fc}\overline{C}_{p,fc}\frac{dT_{fc}}{dt} = \Sigma x_{i,f}\dot{N}_f\overline{C}_{pi,f}(T_{sr} - T_{ref}) + \dot{N}_{air}\overline{C}_{p,air}(T_{air} - T_{ref})$$
$$-\Sigma x_{i,fc}\dot{N}_{fc}\overline{C}_{pi,fc}(T_{fc} - T_{ref}) - x_{H_2,f}\dot{N}_f\Delta H^{\circ}_{r,H_2} - x_{CO,f}\dot{N}_f\Delta H^{\circ}_{r,CO} - V_s I \tag{5}$$

where the subscripts *fc*, *f*, and *air* refer to properties in the outlet stream of SOFC, inlet stream of SOFC, and air inlet stream, respectively; $N_i$, $\dot{N}_i$, and $x_i$ are, respectively, the mole, molar flowrate, and mole fraction of species *i*; $\overline{C}_{pi}$ is the average heat capacity, $\rho_{fc}$ the density of stack, $V_{fc}$ the volume of stack, $\Delta H^{\circ}_r$ the heat of reaction at STP, $V_s$ the cell voltage and $I$ is the current. In Eq. 2 and Eq. 3, I/2F and I/4F refer to the rates of consumption of hydrogen and oxygen by the electrochemical reactions; therefore, the consumption of the reactants is accompanied by the production of water representing the value of I/2F in Eq. 4.

In this paper, the minimization of Gibbs free energy method is exploited to simplify the calculation of the mass balance dynamics of the fuel flow in the SOFC and hydrogen-rich gas production in the steam reformer. Using this method, the equilibrium compositions at the optimum operating conditions of 973 K and $H_2O$:EtOH ratio of 10 giving the maximum hydrogen production are calculated to be 5.38, 7.61, 0.61, 1.38 and 0.004 mol/s of $H_2$, $H_2O$, CO, $CO_2$ and $CH_4$, respectively, when the reactants of ethanol and water are fed to be 1 mol/s and 10 mol/s. Consequently, the temperature dynamics of steam reformer considered to be the heat exchanger, HX1, can be modeled using energy balance as follows:

Cold stream energy balance:

$$\begin{aligned}\rho V_r C_p \frac{dT_{sr}}{dt} &= \dot{N}_{C_2H_6O}\overline{C}_{p,C_2H_6O}(T_{feed}-T_{ref}) + \dot{N}_{H_2O}\overline{C}_{p,H_2O}(T_{feed}-T_{ref}) \\ &-\Sigma x_{i,f}\dot{N}_f\overline{C}_{pi,f}(T_{sr}-T_{ref}) + \Sigma x_{i,f}\dot{N}_f\Delta H_i^f - \dot{N}_{C_2H_6O}\Delta H^f_{C_2H_6O} - \dot{N}_{H_2O}\Delta H^f_{H_2O} \\ &+UA_{HX_1}(T_{HX_1}-T_{ref})\end{aligned} \tag{6}$$

where $\rho$ is the density of reformer, $V_r$ the volume of reformer, $\Delta H_i^f$ the heat of formation of species i and $UA_{HX_1}$ is the overall heat transfer coefficient of HX1.

Hot stream energy balance:

$$\rho_{HX_1,h}V_{HX_1,h}C_{pHX_1,h}\frac{dT_{HX_1}}{dt} = f_{sp}vp_1\dot{N}_{fc}\overline{C}_{p,HX_1}(T_{fc}-T_{HX_1}) - UA_{HX_1}(T_{HX_1}-T_{sr}) \tag{7}$$

where $\rho_{HX_1}$ is the density of HX1, $V_{HX_1}$ the volume of HX1, $f_{sp}$ the constant value of splitter fraction and $vp_1$ is the valve position as the function of time.

Heat exchangers are placed to recover the energy entering from the hot stream. Their energy dynamics are derived by the following equations:

Cold stream energy balance:

$$\rho_{HX_i,c}V_{HX_i,c}C_{pHX_i,c}\frac{dT_c^{out}}{dt} = \Sigma\dot{N}_{ci}\overline{C}_{pi}(T_c^{in}-T_c^{out}) + UA_{HX_i}(T_h^{out}-T_c^{out}) \tag{8}$$

Hot stream energy balance:

$$\rho_{HX_i,h}V_{HX_i,h}C_{pHX_i,h}\frac{dT_h^{out}}{dt} = \Sigma\dot{N}_{hi}\overline{C}_{pi}(T_h^{in}-T_h^{out}) - UA_{HX_i}(T_h^{out}-T_c^{out}) \tag{9}$$

where the *c* and *h* subscripts refer to the cold and hot stream, respectively; the superscripts *in* and *out* refer to the inlet and outlet streams, respectively, and $HX_i$ represents heat exchanger number *i*.

The additional heater is placed before entering the SOFC in order to heat air of inlet stream to be the target temperature of cold stream; therefore, this heater is considered as a hot utility of this integrated system. The energy balance of heater can be written as

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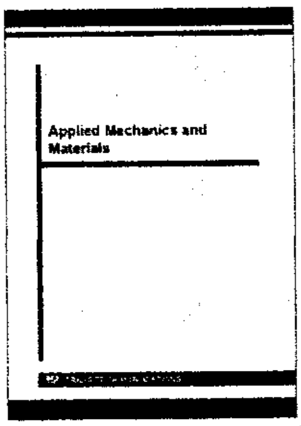


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