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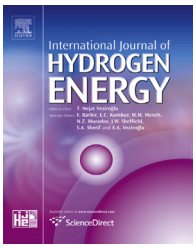

Dynamic modeling of a high-temperature proton exchange membrane fuel cell with a fuel processor

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ABSTRACT

A dynamic model of a high-temperature proton exchange membrane fuel cell with a fuel processor is developed in this study. In the model, a fuel processing system, a fuel cell stack, and an exhaust gas burner are modeled and integrated. The model can predict the characteristics of the overall system and each component at the steady and transient states. Specifically, a unit fuel cell model is discretized in a simplified quasi-three-dimensional geometry; therefore, the model can rapidly predict the distribution of fuel cell characteristics. Various operating conditions such as the steam-to-carbon ratio, oxygen-to-carbon ratio, and autothermal reforming inlet temperature are varied and investigated in this study. In addition, the dynamic characteristics exhibited during the transient state are investigated, and an efficiency controller is developed and implemented in the model to maintain the electrical efficiency. The simulation results demonstrate that the steam-to-carbon ratio and the oxygen-to-carbon ratio affect the electrical and system efficiency and that controlling the fuel flow rate maintains the electrical efficiency in the transient state. The model may be a useful tool for investigating the characteristics of the overall system as well as for developing optimal control strategies for enhancing the system performance.

Introduction

High-temperature proton exchange membrane fuel cells (HT-PEMFCs), which operate in the temperature range of 120–200 °C, have received considerable attention as a promising power generation source in both stationary and mobile systems. Compared with low-temperature proton exchange membrane fuel cells (LT-PEMFCs), HT-PEMFCs have many attractive features, such as simplified water (H_2O) management, no external humidifier installation, increased carbon monoxide (CO) tolerance, and a simplified cooling system [1–11].

Although the direct use of pure hydrogen (H_2) is suitable for operating PEMFC systems, many challenges exist in the production, transportation, and storage of hydrogen due to an insufficient infrastructure [12]. In contrast, the hydrogen produced by reforming hydrocarbon fuel may be an alternative to the successful implementation of fuel cells over the short term. In particular, the methane (CH_4) of natural gas, which is usually used for reforming, is abundant and easily supported by established infrastructures [13]. In addition, HT-

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Nomenclature

A	convective efficient area per volume, 1 m^{-1}, surface area, m^2
C	solid specific heat capacity, kJ kg^{-1} K^{-1}, concentration, kmol
C_V	gas constant-volume specific heat capacity, kJ kg^{-1} K^{-1}
E	energy, kW
E_a	activation energy, kJ $kmol^{-1}$
F	Faraday's constant, 96,485 C mol^{-1}
HEX	heat exchanger
h	enthalpy, kJ $kmol^{-1}$, convective heat transfer coefficient, kW m^{-2} K^{-1}
I	electrical current, A
i_0	exchange current density, A m^{-2}
LHV	lower heating values
N	total number of moles, kmol
$\dot{N}$	molar flow rate, kmol s^{-1}
P	power, kW
$\dot{Q}$	heat, kW
R	gas constant, 8.31 J K^{-1} mol^{-1}, fuel cell external/load resistance, Ω
t	time, s
T	temperature, K
V	voltage, V
$\forall$	volume, m^3
$\vec{X}$	species mole fraction, –

Greek letters

α	transfer coefficient, –
η	efficiency, –, overvoltage, V
κ	ionic conductivity, S m^{-1}
ρ	density, kg m^{-3}
σ	electrode conductivity, S m^{-1}
$\vec{\Phi}$	species diffusion flux between GDL and bulk gases, kmol s^{-1}

Superscripts and subscripts

act	activation polarization
c	catalyst control volume
elec	electricity
GDL	gas diffusion layer
g	gas control volume
gc	from gases to catalyst
gas	gas process
in	into control volume
inlet	inlet of the fuel processor
MEA	membrane electrode assembly
out	out of control volume
ref	reference condition
stack	fuel cell stack
0	standard condition

PEMFCs have a high tolerance for CO; therefore, hydrogen, which contains impurities after the reformation of hydrocarbon fuel, is suitable for the system without exerting a severe poisoning effect on the catalyst layer [14].

To use methane as an energy source for the fuel cell, a fuel processor is needed to convert methane into hydrogen and reduce the CO concentration in the fuel cell to a certain level. Thus, the fuel processor mainly consists of a reforming section and a clean-up section. In the reforming section, there are several ways to reform the hydrocarbon fuel: steam reforming (SR), catalytic partial oxidation (CPO), and autothermal reforming (ATR). In the clean-up section, there are water-gas-shift (WGS) and preferential oxidation (PrOx) reactors to reduce the CO [15–18].

To date, system level dynamic modeling studies on HT-PEMFCs have been limited compared with those on LT-PEMFCs even though system-level modeling is useful for improving system integration and understanding the system behavior under transient operating conditions. Conversely, several component-level modeling studies on HT-PEMFCs have been reported. Cheddie and Munroe [19–21] developed a steady-state one-dimensional HT-PEMFC model as well as a multi-dimensional model in the early stages of HT-PEMFC modeling studies. Peng and Lee [3] developed a three-dimensional steady-state non-isothermal numerical model with a computational fluid dynamics (CFD) code. Then, these authors incorporated the aforementioned model into a dynamic model and investigated the charge double-layer effect. Additionally, Sousa et al. [22] developed a dynamic two-dimensional non-isothermal model and observed the double-layer effect. Su et al. [23] developed a three-dimensional CFD HT-PEMFC model and considered the effects of various operating parameters, such as the inlet gas temperature, system pressure, and inlet gas flow rate, on the performance. Jiao et al. [24] developed a three-dimensional non-isothermal model and investigated the combined effects of the flow channel design and CO poisoning on the performance. Using a the quasi-three-dimensional non-isothermal dynamic model, our research group [25] observed that the transient response of the voltage is strongly dependent on the cell temperature. These HT-PEMFC models only focus on the HT-PEMFC component; therefore, the models cannot predict the characteristics of fully integrated HT-PEMFC systems. Furthermore, most of these modeling studies have only reported the observation of steady-state characteristics, although understanding the transient behavior of the system is essential.

For fuel processor system modeling, most studies conducted to date have focused on the reactor design or reaction kinetics. Francesconi et al. [26] developed a one-dimensional heterogeneous model of a WGS reactor and optimized the design variables for such reactors. Choi et al. [27] formulated the empirical kinetic rate equation of a WGS reactor, which fit experimental data with good accuracy, and applied the equation to a simple isothermal plug flow model. Zalc et al. [18] applied basic chemical engineering principles to the model and simulated the effect of the reactor design and size for each component of the fuel processor. Although most modeling studies have focused only on fuel processor systems, a few have considered the entire PEMFC system. Lattner et al. [17] developed a LT-PEMFC system model using Aspen-HYSYS® and compared SR, ATR, and ATR membrane reactor-based fuel processors in terms of their overall system efficiencies. In