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Modeling and operation optimization of a proton exchange membrane fuel cell system for maximum efficiency

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ABSTRACT

This paper presents an operation optimization method and demonstrates its application to a proton exchange membrane fuel cell system. A constrained optimization problem was formulated to maximize the efficiency of a fuel cell system by incorporating practical models derived from actual operations of the system. Empirical and semi-empirical models for most of the system components were developed based on artificial neural networks and semi-empirical equations. Prior to system optimizations, the developed models were validated by comparing simulation results with the measured ones. Moreover, sensitivity analyses were performed to elucidate the effects of major operating variables on the system efficiency under practical operating constraints. Then, the optimal operating conditions were sought at various system power loads. The optimization results revealed that the efficiency gaps between the worst and best operation conditions of the system could reach 1.2–5.5% depending on the power output range. To verify the optimization results, the optimal operating conditions were applied to the fuel cell system, and the measured results were compared with the expected optimal values. The discrepancies between the measured and expected values were found to be trivial, indicating that the proposed operation optimization method was quite successful for a substantial increase in the efficiency of the fuel cell system.

1. Introduction

Fuel cells have been actively studied for the last several decades because they have been regarded as the most promising alternatives to conventional power generation systems such as internal combustion engines and gas turbines [1,2]. Several types of fuel cells, including solid oxide fuel cells (SOFCs), phosphoric acid fuel cells (PAFCs), molten carbonate fuel cells (MCFCs), direct methanol fuel cells (DMFCs), alkaline fuel cells (AFCs), and proton exchange membrane (PEM) fuel cells, have been commercialized for various applications [3]. Their working principles, advantages and disadvantages have been well explained in various references including a textbook [4]. Among these, PEM fuel cells are suitable for both stationary and transportation applications such as residential power generators, cars, buses, forklifts, bicycles, and watercraft because they offer many advantages, including high efficiencies, high power densities, short startup times, and low emissions of pollutants [5].

As fuel cell systems have spread, the need for their operational optimization to heighten performance or reduce operating costs has gained increased attention. To maximize the efficiency of a fuel cell system, and thereby minimize its operating cost, it is essential that it operates near its optimal operating conditions. This can be usually achieved by performing operation optimization techniques based on mathematical models [6]. However, the model-based optimization of a fuel cell system is a challenging task because accurate models for all its components must be available in order to find real optimal operating conditions that will deliver a substantial improvement in performance. A number of papers dealing with the operation optimizations of fuel cells have been published in the open literature. However, most have focused on the optimization of single components [7–12] or sub-systems [13–15] rather than complete systems [16–22].

A considerable number of papers on the operation optimization of single fuel cells or sub-systems have been published. Mawardi et al. [7] proposed a model-based optimization to maximize the power density of a single PEM fuel cell. Meidanshahi and Karimi [8] performed an optimization study using a one-dimensional dynamic model for a single PEM fuel cell. Zhang et al. [9] determined the optimal operating temperature of a high-temperature PEM fuel

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Nomenclature

$\mathbf{b}$	bias vector in an artificial neural network model
C_{pw}	heat capacity of the cooling water (4.186 kJ kg^{-1} K^{-1}).
F	flow rate (SLPM)
$F_{H_2}^{stoic}$	stoichiometric flow rate of hydrogen entering the stack (SLPM)
F_{purge}	purge gas flow rate from the stack (SLPM)
f	transfer function of an artificial neural network model
$\tilde{F}$	Faraday constant (96,485 C mol^{-1})
g	transfer function of an artificial neural network model
I	current (A)
J	objective function (%)
MW_a	molecular weight of air (28.97 kg kg-mol^{-1})
N_s	number of cells in the stack
P	pressure (gauge pressure in kPa)
P_a	discharge pressure of the air from the air blower (gauge pressure in kPa)
P_e	ambient pressure (gauge pressure in kPa)
R	universal gas constant (8.314 J mol^{-1} K^{-1})
RMSE	root mean squared error defined by $\sqrt{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2/n}$ where n is the number of measurements, y_i the measured variable, and $\hat{y}_i$ the predicted variable
R^2	coefficient of determination
T	temperature (°C)
V_{cell}	average cell voltage of the stack (V)
W	power (kW)
W_{demand}	power demand of the electricity users (kW)

Greek letters

γ_a	mean adiabatic exponent of air (1.402)
ΔT	temperature difference (°C)
ΔT_{g-wa}	temperature difference between the exhaust gas and the humidified air (°C)
η	efficiency (%)
η_{fuel}	fuel utilization efficiency of the stack (%)
$\boldsymbol{\theta}$	vector of the decision variables
ρ_w	density of the cooling water (0.981 kg L^{-1})
$\boldsymbol{\omega}$	weight matrix in an artificial neural network model

Subscripts

A	air blower
a	air
B	pump and other balance of plants
c	cooling water
g	exhaust gas exiting the cathode of the stack
P	power converter
S	stack
T	fuel cell system
wa	humidified (wet) air to the stack

Superscripts

HL	hidden layer of an artificial neural network model
in	power input
lb	lower bound
max	maximum
min	minimum power
OL	output layer of an artificial neural network model
out	power output
ub	upper bound

cell by considering its performance, CO tolerance, and durability. Kanani et al. [10] used a response surface method to maximize the power output of a single PEM fuel cell. Ni et al. [11] carried out a parametric study using an electrochemical model to elucidate the effects of operating variables on the performance of a single SOFC. Tafaoli-Masoule et al. [12] employed a genetic algorithm and a quasi two-dimensional, isothermal model to determine the optimal operating temperature and pressure of a single DMFC. Subramanyan et al. [13] performed a multi-objective optimization for a hypothetical SOFC–PEM hybrid sub-system both to minimize the CO_2 emission and to maximize the performance. Caliandro et al. [14] presented a multi-objective optimization for a SOFC–GT (gas turbine) hybrid sub-system both to maximize the efficiency and to minimize the capital costs. Ranjbar et al. [15] analyzed the effects of operating variables on the energy and exergy efficiencies of a hybrid SOFC sub-system, using a zero-dimensional mathematical model.

Several papers on system-level operation optimizations of PEM fuel cells have appeared in the open literature. Godat and Marechal [16] performed a simulation study to find the optimal process structure and operating conditions for a stationary fuel cell system consisting of a PEM fuel cell stack and fuel processing units. They analyzed the sensitivity of the major decision parameters (the steam-to-carbon ratio, reforming and cell temperatures, and fuel utilization) on the overall efficiency of the fuel cell system. Bao et al. [17] carried out an optimization study for a hypothetical PEM fuel cell system, using a hybrid model that combined a neural-network model with a first-principles model, to find the optimal operating conditions that maximized net power generation. The optimal values of two operating variables (the air stoichiometry and cathode outlet pressure) were sought using a genetic algorithm under three different configurations of the air-supply system. Wu et al. [18] presented an optimization approach to find the optimal operating conditions for a 25-cm^2 single PEM fuel cell coupled with a hypothetical compressor and a humidifier. They employed a meta-modeling approach in which the input-output relations were approximated with radial basis functions (RBFs) using the data obtained from a simulator, to reduce the computational burden in locating an optimal solution. Four decision variables—the cell temperature, cathode stoichiometry, cathode gas pressure, and cathode relative humidity—were sought under ideal and realistic system assumptions after accomplishing a model validation for the fuel cell. Hasikos et al. [19] adopted a dynamic first-principles model, which was originally proposed by Pukrushpan et al. [23], as a hypothetical PEM fuel cell system composed of a stack and auxiliary units to generate operational data for optimizations. A meta-modeling approach was employed to build the optimization models from the operational data using an RBF neural network. They formulated an optimization problem to minimize the stack current at a given power demand, and then the optimal operating conditions were used as set-points for the dynamic matrix controls (DMCs) of the hypothetical system. Wishart et al. [20] performed a system-level optimization for an experimental system comprising a Ballard Mark IV fuel cell stack, a compressor, and pumps. They demonstrated two different optimization cases to find the optimal operating conditions for vehicular and stationary applications. Mert et al. [21] presented an optimization of a PEM fuel cell system for vehicular applications. They carried out a multi-objective optimization of the vehicular fuel cell system both to maximize the power output, energy, and exergy efficiencies and to minimize the cost of the produced work. A simple electrochemical model for a Ballard Xcellsis™ HY-80 fuel cell engine was employed for the optimization. Frangopoulos and Nakos [22] performed optimization simulations for