Journal of Power Sources 185 (2008) 345–355

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Development of a novel computational tool for optimizing the operation of fuel cells systems: Application for phosphoric acid fuel cells

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ARTICLE INFO

Article history:
Received 29 February 2008
Received in revised form 19 May 2008
Accepted 22 June 2008
Available online 9 July 2008

Keywords:
Fuel cells
CFD
Modeling
Optimization
Neural networks

ABSTRACT

Fuel cells offer a significant and promising clean technology for portable, automotive and stationary applications and, thus, optimization of their performance is of particular interest. In this study, a novel optimization tool is developed that realistically describes and optimizes the performance of fuel cell systems. First, a 3D steady-state detailed model is produced based on computational fluid dynamics (CFD) techniques. Simulated results obtained from the CFD model are used in a second step, to generate a database that contains the fuel and oxidant volumetric rates and utilizations and the corresponding cell voltages. In the third step mathematical relationships are developed between the input and output variables, using the database that has been generated in the previous step. In particular, the linear regression methodology and the radial basis function (RBF) neural network architecture are utilized for producing the input–output "meta-models". Several statistical tests are used to validate the proposed models. Finally, a multi-objective hierarchical Non-Linear Programming (NLP) problem is formulated that takes into account the constraints and limitations of the system. The multi-objective hierarchical approach is built upon two steps: first, the fuel volumetric rate is minimized, recognizing the fact that our first concern is to reduce consumption of the expensive fuel. In the second step, optimization is performed with respect to the oxidant volumetric rate. The proposed method is illustrated through its application for phosphoric acid fuel cell (PAFC) systems.

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1. Introduction

A fuel cell is a device where chemical energy from a fuel, such as hydrogen, is electrochemically converted to electrical and thermal energy, without the need for combustion and without producing noise or pollution. Performance optimization is a primary target of the fuel cell technology that can substantially increase its competitiveness and benefits in industrial, automotive and environmental applications.

Fuel cells offer a significant and promising clean technology, but they are governed by complex multi-physics phenomena, that can be modeled only by advanced modeling tools. Among several alternative techniques, computational fluid dynamics (CFD) models have been used extensively for simulating the static and/or dynamic operation of fuel cells [1–4]. However, most modeling techniques suffer from long simulation running times. Mathematical meta-models based on CFD results [5] can noticeably increase simulation speed. Neural network models (NNM) have been used with success to develop such meta-modeling relationships between input and output variables [6]. Recent research has shown that neural network approaches can produce simulation results of high accuracy and reliability, whereas at the same time the computational times are reduced significantly [7,8]. Moreover, NNM applications are considered as a practical and alternative methodology to analytical and empirical models of fuel cells [9].

In this paper, we present a novel method for examining and optimizing the performance of fuel cell systems based on a meta-modeling approach. Initially, a detailed 3D steady-state, isothermal CFD simulation model [10] of the fuel cell system is used to generate a database that contains the values of the key system variables: the fuel and oxidant volumetric rates and utilizations and the

Abbreviations: 3D, three-dimensional; CFD, computational fluid dynamics; CPU, central processor unit; FC, fuel cell; LHV, lower heating value; LOO, leave one out; NLP, Non-Linear Programming; NNM, neural network model; OCV, open circuit voltage; PAFC, phosphoric acid fuel cell; PEMFC, proton exchange membrane fuel cell; PRESS, prediction error sum of squares; RAM, random access memory; RBF, radial basis function; RMSE, root mean-squared error; SOFC, solid oxide fuel cell; SSE, sum of squared errors between the observations and the predicted values; SSY, sum of squared deviations between the observations and their mean; STP, standard temperature and pressure conditions.

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doi:10.1016/j.jpowsour.2008.06.081

Nomenclature

A	Tafel constant (V)
A_{eff}	electrode effective area (m^2)
C_i	concentration of component i, where i are components of a gas mixture ($kg_i\ kg_{mix}^{-1}$)
$D_{i,\text{mix}}$	mixture molar diffusivity ($m^2\ s^{-1}$)
D_{ij}	binary diffusivities for each pair of chemical species in gas mixture ($m^2\ s^{-1}$)
E	reversible open circuit voltage given by Nernst equation (V)
I	current density ($A\ m^{-2}$)
I^*	optimal value of current density ($A\ m^{-2}$)
I_0	exchange current density ($A\ m^{-2}$)
k	number of independent variables
L	number of hidden nodes in the neural network topology
m	constant in the empirical equation for mass concentration losses (V)
$m_{H_2,\text{input}}$	mass of fuel input in cell ($kg\ s^{-1}$)
$m_{H_2,\text{react}}$	mass of fuel reacted in cell ($kg\ s^{-1}$)
$m_{O_2,\text{input}}$	mass of oxidant reacted in cell ($kg\ s^{-1}$)
$m_{O_2,\text{react}}$	mass of oxidant input in cell ($kg\ s^{-1}$)
n	number of the available data
n_c	constant in the empirical equation for mass concentration losses ($m^2\ A^{-1}$)
n_{eff}	fuel cell efficiency (%)
n^*_{eff}	optimal value of fuel cell efficiency (%)
P_C	fuel cell output power (W)
P_D	power demand (W)
PD	power density ($W\ m^{-2}$)
PD*	optimal value of power density ($W\ m^{-2}$)
Q_f	inlet fuel gas volumetric rate ($l\ h^{-1}$)
Q_f^1	value of the inlet fuel gas volumetric rate after the first stage of the optimization problem ($l\ h^{-1}$)
Q_f^*	optimal value of the inlet fuel gas volumetric rate ($l\ h^{-1}$)
Q_{ox}	inlet oxidant gas volumetric rate ($l\ h^{-1}$)
Q_{ox}^*	optimal value of the inlet oxidant gas volumetric rate ($l\ h^{-1}$)
r	area specific resistance ($\Omega\ m^{-2}$)
R^2	coefficient of determination (%)
R^2_{CV}	coefficient of determination by using the cross-validation technique (%)
S_ϕ	source term of ϕ variable
$\vec{u}$	velocity vector
U_f	hydrogen utilization (%)
U_f^*	optimal value of hydrogen utilization (%)
U_{ox}	oxygen utilization (%)
U_{ox}^*	optimal value of oxygen utilization (%)
V_C	cell voltage (V)
$\bar{V}_C$	mean of all CFD cell voltage values in the available dataset
V_C^*	optimal value of cell voltage (V)
$V_{C,i}$	CFD cell voltage value for observation i (V)
$\hat{V}_{C,i}$	model prediction of cell voltage for observation i (V)
$\hat{V}^{\text{LOO}}_{C,i}$	cell voltage prediction for observation i of the model that is trained using all the available data, except for observation i
ΔV_{act}	activation losses (V)
ΔV_{conc}	concentration losses (V)
ΔV_{losses}	cell voltage losses (V)
ΔV_{ohm}	ohmic losses (V)
w_j	the weight corresponding to the response of the jth node in the neural network topology
$\mathbf{x}_j$	the centre of the jth node in the neural network topology
$\mathbf{x}$	input vector in the neural network model
X_j	Molar fraction of mixture component j
z_j	The response of the jth node in the neural network topology

Greek symbols

α	charge transfer coefficient (typical value 0.5)
β_f	coefficient in the definition of hydrogen utilization
β_{ox}	coefficient in the definition of oxygen utilization
Γ_ϕ	exchange coefficient
Γ_{C_i}	exchange coefficient representing the diffusivity for each mixture component ($kg\ m^{-1}\ s^{-1}$)
θ	tuning parameter in the formulation of the multi-objective optimization problem
μ_{mix}	viscosity of the mixture (Pa s)
ρ	density of the mixture ($kg\ m^{-3}$)
ϕ	dependent variable, i.e. U, V, W, C_i, and 1 for continuity

corresponding cell voltages. These values are obtained after several runs of the CFD model. Linear regression is then applied to develop a linear correlation model between the input and the output variables, while an advanced NNM methodology is applied to obtain a non-linear model. The database is also used for validating the accuracy of both linear and non-linear models. Eventually, a hierarchical multi-objective optimization problem is formulated, that can be used with both linear and non-linear approaches, in order to obtain the optimal values of the decision variables, i.e. the fuel and oxidant volumetric flows. The proposed computational tool is illustrated through its application for phosphoric acid fuel cell (PAFC) systems and is summarized graphically in Fig. 1.

2. PAFC simulation

2.1. CFD modeling

2.1.1. The physical problem

PAFCs belong to the medium operation temperature fuel cells (~220 °C). The type of the electrolyte that is used in a PAFC permits and facilitates the conduction of mobile H^+ ions. Air or pure oxygen is used as the oxidant gas, while pure hydrogen or a gas mixture that contains hydrogen and carbon dioxide (produced by hydrocarbon reforming) is used as fuel gas.

Reactions taking place in a PAFC are the following:

$$\textit{Anode}: \quad 2H_2 \rightarrow 4H^+ + 4e^- \tag{1}$$

$$\textit{Cathode}: \quad O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \tag{2}$$

$$\text{Total reaction}: \quad H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \tag{3}$$

In the PAFC system considered in this work, the content of the anode electrode is 10 wt% Pt/C of catalyst powder, while for the cathode the catalyst powder used contains 25 wt% Pt/C. The fuel gas and the oxidant gas enter the PAFC in cross-flow. The fuel gas flows in the longer electrode and the oxidant gas in the shorter one, when an orthogonal cell is considered. The examined fuel cell geometry is given in Table 1.

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