Optimization of the Operating Parameters of a Proton Exchange Membrane Fuel Cell for Maximum Power Density

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The performance of fuel cells can be significantly improved by using optimum operating conditions that maximize the power density subject to constraints. Despite its significance, relatively scant work is reported in the open literature on the model-assisted optimization of fuel cells. In this paper, a methodology for model-based optimization is presented by considering a one-dimensional nonisothermal description of a fuel cell operating on reformate feed. The numerical model is coupled with a continuous search simulated annealing optimization scheme to determine the optimum solutions for selected process constraints. Optimization results are presented over a range of fuel cell design parameters to assess the effects of membrane thickness, electrode thickness, constraint values, and CO concentration on the optimum operating conditions.
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1 Introduction

Proton exchange membrane (PEM) fuel cells are a promising technology for a wide variety of application of power generations. Power sources consisting of PEM fuel cells have the advantages of low operating temperature and pressure, quick start-up, and pollution-free operation [1]. The overall cell performance is governed by the critical issues of water and thermal management [2–7]. Since the membrane in a PEM fuel cell requires sufficient water content to maintain desired ionic conductivity, the fuel and oxidant streams are commonly humidified. However, excessive water from the feed streams and the electrochemical reaction will flood the electrode pores, which degrades the fuel cell performance by preventing the reactants from reaching the catalyst sites. In general, higher operating temperature is desirable to decrease mass transport losses and to increase the electrochemical reaction rates; at the same time, the increase in water vapor pressure with increasing temperature results in increased mass transport losses.

Extensive studies on modeling and computer simulation of PEM fuel cells have been conducted toward better understanding the transport and electrochemical processes. Bernardi and Verbrugge [8,9], Springer et al. [10,11], Baschuk and Li [12], and Rowe and Li [13] developed one-dimensional models for steady state operation of fuel cells, assuming perfect membrane hydration. Amphlett et al. [14,15] studied the transient response of a fuel cell stack by performing a global heat and mass balance analysis, and the details of electrochemical phenomena inside the cell were ignored. Two-dimensional modeling of transport phenomena in PEM fuel cells was presented by Gurau et al. [16], Um et al. [17], Wang et al. [18], You and Liu [19] and You [20], where two phase flows in the fuel cell systems were also discussed.

The performance of the fuel cells can be significantly improved through model-based optimization studies. To the knowledge of the authors, however, little effort has been made to systematically determine the optimum conditions for fuel cell systems. Mishra et al. [21] illustrated a methodology for model-based design and optimization of the operating parameters based on a comprehensive parametric analysis on the various physical and electrochemical phenomena. Specific optimization solutions were obtained by changing one of the operating or design parameters while fixing the values of the remaining ones. This paper provides an optimization framework to derive more general optimum solutions. The objective of the optimization is to determine the optimum operating parameters for maximizing the power density, and simultaneously satisfying constraints on (*a*) the maximum temperature difference across the cell, $\Delta T_{\max}$, (*b*) the minimum membrane hydration, $\lambda_{\min}$, and (*c*) the cell potential, Φ. A numerical simulation model for fuel cells on reformate feed is adopted in this study [21] to obtain the information on objective function and constraints, which, in turn, is combined with a simplex search based simulated annealing optimizer to obtain the optimum operating conditions.

The paper is organized as follows: The process model is briefly described in the next section, followed by a discussion of the mathematical formulation of the optimization problem in Sec. 3. Numerical results are presented in Sec. 4 for six fuel cell design cases to illustrate the effects of cell component geometries, constraint values, and carbon monoxide concentration on the optimum solutions.

2 Mathematical Model of a PEM Fuel Cell

To introduce the framework for model-based optimization of a PEM fuel cell, a physical model for the transport and electrochemical phenomena is needed. To this end, a comprehensive model from Mishra et al. [21] is adopted to predict the performance of a PEM fuel cell operating on reformate feed. The model considers a typical PEM fuel cell, where a polymer membrane is placed between an anode and a cathode electrode to form a membrane electrode assembly (MEA). Two bipolar plates housing the flow channel are used to clamp the MEA, as shown in Fig. 1. Thin catalyst layers exist between each of electrodes and the membrane, referred to as the anode and cathode catalyst layer, respectively. The cell is considered to be operating at steady state, and since the primary aim of the study is to present a framework for optimization of cells using physics-based models, the discussion is limited to a one-dimensional modeling in the direction along the cell thickness. The modeling further includes the effects of carbon monoxide (CO) poisoning of the catalysts, as is prevalent in fuel cells operating on a reformate feed, but is often neglected in fuel cell modeling. In the electrode regions, since the viscous force and

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