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Estimation of Optimum Operating Profile for PEMFC

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In this paper, we present a methodology to estimate the optimum operating condition for increasing the available power density from the Proton Exchange Membrane Fuel cell (PEMFC). This is achieved by implementing an optimization procedure on a mathematical model of the PEMFC. As a first step, the input condition in steady state is optimized and dynamic optimization is implemented on the transient model. It was observed that the first-principles model requires large computational time and hence we propose to reformulate the model to increase the computational efficiency and then use the same for dynamic optimization.

Introduction

Typically, fuel cells are operated to deliver maximum power, and operating conditions are decided from the polarization curve, which is a steady state representation of the system. However, due to various dynamics taking place in the system, operating conditions chosen from the polarization curve might not be sufficient to provide the required optimum performance of the cell. The fact that the operating temperature of the PEMFC changes with time, actually affects the cathode and anode gas temperatures, which in turn affect the rate of condensation/vaporization of water vapor at the cathode and anode. Due to the change in concentration of water at the membrane, the direction as well as magnitude of the transportation of protons is affected. This in turn affects the production of current from the PEMFC. Many such known/unknown phenomena take place in PEMFC, which results in the decrease in overall efficiency of the PEMFC.

There are various potential manipulated variables in PEMFC [1], of which some are more effective toward attaining the required power density from the fuel cell. To increase the efficiency of PEMFC, it is critical to operate it at optimal operating conditions. This can be achieved either by designing a control algorithm for PEMFC and force the system dynamics to follow an optimal operating condition or to estimate the optimal operating condition by implementing dynamic optimization. In literature, a number of attempts have been reported for maintaining a PEMFC at the optimal condition by designing the control algorithms based on reduced order models, empirical models or using model identification procedure (identifying simpler models). Nevertheless, to our knowledge, control and optimization of PEMFC using full-order physics based model directly have not been reported.

The key component of control/optimization scheme is the dynamic model used for optimization and control. To address the complex nonlinear dynamics of the PEMFC, researchers have used two/three dimensional physics based models. [2, 7] But these types of models in general, are computationally very expensive and hence may not be useful in designing the control or optimization algorithm.

To optimize the operating conditions for the efficient use of PEMFC there is a need to have computationally efficient models comprehensive enough to capture the entire nonlinear dynamics-taking place in the system. We have recently developed and

implemented a model reformulation approach to develop physics based efficient models (CPU time < 15 ms) for lithium-ion batteries [6]. From our experience in the battery domain, we believe that model reformulation approach will be useful for finding computationally efficient physics based models for the PEMFC.

In this paper, as a first step, we simulated the steady state one-dimensional model of the PEMFC given by Nguyen and White [4], and simulated by Methekar *et al*. [1] After successfully simulating the model, an objective function was constructed which will maximize the power obtained from the fuel cell in steady state. Then, this objective function was solved to obtain the optimum input conditions of the various manipulated variables. Further, we optimized the power obtained from the fuel cell in transient conditions. However, the present model being used requires very high computation time to be used in a dynamic optimization algorithm.

Distributed Parameter Model of the PEMFC

This model accounts for *i)* the reactions taking place at the anode and cathode, *ii)* heat transfer taking place between the solid and the two gas channels, and *iii)* heat transfer between the solid and coolant. The dynamics of the systems are captured through the energy balance equations. The electrochemical reactions are known to be faster than the temperature dynamics and hence all other equations except the energy balance are assumed to be at quasi-steady state for a given solid temperature profile. To avoid the dehydration at the anode, the anode and cathode streams are saturated with water vapor. For the sake of brevity, we are not providing the modeling equations and initial base conditions, but interested readers may refer the literature such as Nguyen and White, Methekar *et al*. and Golbert and Lewin [4, 1, and 5].

Static Optimization

Effects of Changing the Initial Conditions

Methekar *et al.* suggest that PEMFC have many potential manipulated variables such as inlet molar flow rate of hydrogen and oxygen, inlet gas temperature at the cathode and anode, cell voltage or current. They also suggested that some of the above-described manipulated variables have positive gain with power density and some of them have negative gain. Figure [1] shows the effects of the change in hydrogen flow rate, cathode and anode gas temperature and voltage on the power density. It is observed that power density decreases with an increase in voltage upto certain range and then vice versa. The cathode gas temperature is inversely proportional to the power density whereas hydrogen flow rate and anode gas temperature are directly proportional within the physical limits of the process variables. Now if one can fix the input conditions using the stoichiometry, without considering the interaction of all the possible manipulated variables, it might be possible that PEMFC would operate at suboptimal operating conditions and hence may decrease the efficiency the PEMFC. To avoid this, it is necessary to estimate an optimum operating condition of the PEMFC. In the next section, we have described the formulation of an objective function and its solution for optimum operating conditions.

Estimation of Optimum Operating Conditions

In general, dynamic optimization for any system can be written as

$$\min_{\mathbf{z}(t),\mathbf{u}(t),\mathbf{p}} \Phi(\mathbf{z}(t_f))$$

$$s.t. \frac{d\mathbf{z}}{dt}(t) = \mathbf{f}(\mathbf{z}(t), \mathbf{y}(t), \mathbf{u}(t), \mathbf{p}), \quad \mathbf{z}(t_0) = \mathbf{z}_0 \qquad [1]$$

$$\mathbf{g}(\mathbf{z}(t), \mathbf{y}(t), \mathbf{u}(t), \mathbf{p}) = 0 \ , \ \mathbf{g}_f(\mathbf{z}(t_f)) = 0$$

$$\mathbf{u}_L \le \mathbf{u}(t) \le \mathbf{u}_U \quad \mathbf{y}_L \le \mathbf{y}(t) \le \mathbf{y}_U \quad \mathbf{z}_L \le \mathbf{z}(t) \le \mathbf{z}_U$$

Where the vectors represent the differential state variables **z** (t), algebraic variables **y** (t), control variables **u** (t), all functions of parameters **p**. In the PEMFC problem, our aim is to obtain maximum power density by controlling the manipulated variables such as inlet molar flow rate of hydrogen, coolant, inlet gas temperature at cathode and anode and cell voltage.

The optimum operating condition in steady state was estimated and hence we call it static optimization. In static optimization, the physics based model is solved at steady state the current density is obtained along the channel, and then power density is calculated by multiplying the average current density with the cell voltage. The objective function is formed such that the power obtained from the fuel cell is maximized based on the initial conditions of the chosen control variables. Then the optimized operating condition is supplied to the model and the optimized current density is estimated. Figure [2] shows a comparison between the estimated optimized current density and the un-optimized current density along the channel. Figure [2] demonstrates that the optimized current density is higher than the un-optimized current density. An increase in current density along the channel is observed because of the proper selection of input conditions. The objective function while selecting the input conditions has considered the various interactions of the manipulated variables, which would not have been possible by merely selecting the input conditions using only the stoichiometric knowledge.

Dynamic Optimization

Dynamic optimization for the given model with the solution procedure described by Methekar *et al*., takes approximately 24 hours on 3 GHz CPU with 16 GB RAM. Hence, it is extremely important to perform model reformulation to increase the computational efficiency there by reducing the simulation time. Model reformulation for the PEMFC is currently in progress and will be reported at a later stage by the authors.

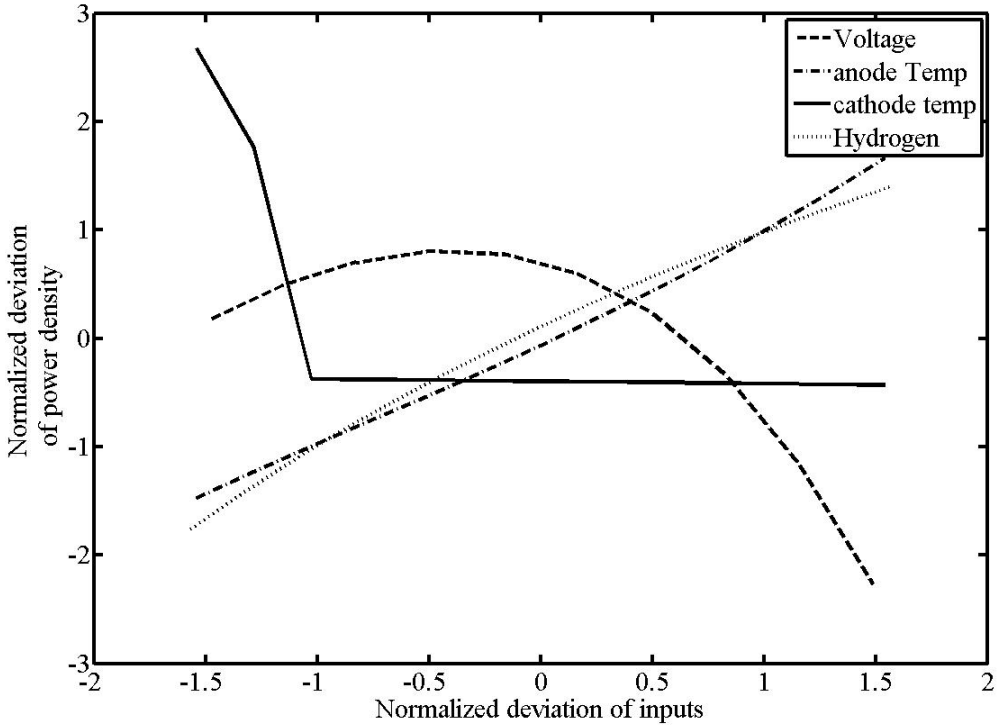

Figure (1): Effects of changing the initial conditions (Cell voltage, anode and cathode temperature and hydrogen flow rate) on the average power density.

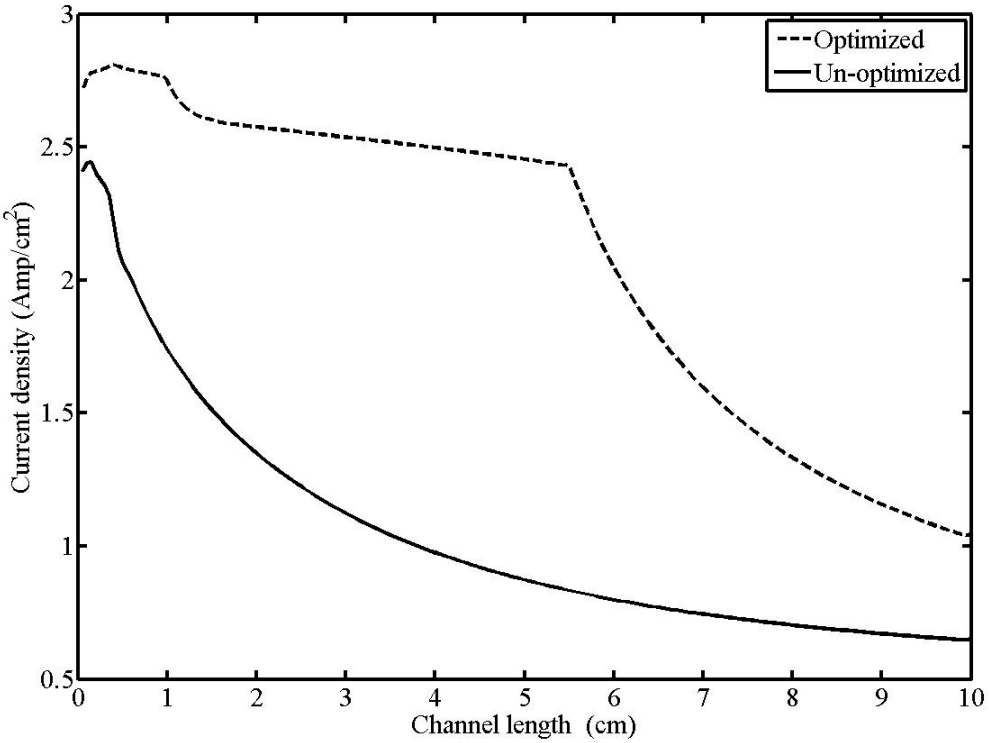

Figure (2): Change in current density along the channel (optimized and un-optimized case).

Acknowledgments

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