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Effects of water induced pore blockage and mitigation strategies in low temperature PEM fuel cells – A simulation study

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ABSTRACT

Ineffective water management in proton exchange membrane fuel cells (PEMFCs) can cause performance degradation. A simple mathematical model capturing the effect of water on the overall performance of the fuel cell system is of immense use in developing tools for water management. In this work, a computationally efficient first principles dynamic model for PEMFC system simulations and concomitant water management studies are developed. The steady-state version of this model is validated with experimental data. The effect of various operating conditions and design parameters on the performance of the fuel cell is studied using this model. Various control strategies for improving fuel cell performance in the presence of flooding are evaluated using the model. The simplicity and adequate predictive capability of the model make it amenable to be used in a model-based feedback control framework for online water management.

Introduction

Polymer electrolyte membrane (or) proton exchange membrane fuel cell (PEMFC) is one of the highly researched fuel cell types due to its applications in automotive, stationary and small scale power devices [1,2]. Fuel cells convert chemical energy to electrical energy directly by utilizing the reaction between H_2 and O_2 producing water as the end product, which makes them attractive as an environment friendly energy source. Fuel cell models are essential to understand the functioning of fuel cells and in estimating their power output.

First principles models of PEMFCs allow us to understand and comprehend the complex processes occurring in the fuel cells, which include mass and heat transfer, electrochemical reactions, ionic and electronic transport. These models can be used as theoretical laboratories for virtually testing various possible designs, operational conditions, and extracting information to enhance the performance of fuel cells. A fundamental understanding of the underlying physics and experimental observations form the basis of any model. Thus, fuel cell models can be mechanistic (accounting the physics for various processes in fuel cells) or empirical (equations fitted to experimental data). In terms of dimensional complexity, fuel

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cell models range from zero dimensional (0-D) to three dimensional (3-D) and account, in general, for transport processes, electrochemical reactions, water and thermal management. Computational fluid dynamics based models, which help in flow visualization and design studies have also gained popularity with the advent of high power computing in recent years [3–5].

Several models have been developed in literature to understand the performance of fuel cells and a classification of these models has been provided by Weber and Newman in their review [1]. Two important models that were developed initially were that of Bernardi and Verbrugge [6], and Springer et al. [7]. These models have been improved subsequently by several other researchers to include various processes leading to an increase in their levels of detail. To elaborate, Bernardi and Verbrugge's model considers a fully hydrated membrane, porous electrodes, and Stefan–Maxwell type multicomponent diffusion in GDL and catalyst layers. Also, Bernardi [8] developed a simpler study emphasizing the importance of water management and its effect on the performance of fuel cells. The paper also examined the effect of operating conditions such as temperature, pressure and gas humidity on water balance in the fuel cell. On the contrary, Springer's model was 0-D isothermal model which considered the polarization and electrode effects. Overall, these models and their derivatives have been used to study various factors such as catalyst utilization, gas diffusion layer (GDL) porosity effects, proton conductivity, material composition effects, humidification, transport properties, water balance, multi-phase flow and other transient processes in fuel cell systems, to mention a few [9–13]. Models focusing on different PEM fuel cell geometries and various catalyst layer designs have been developed recently by Srinivasarao et al. [14–17]. Additionally, detailed analytical models of fuel cells and mechanistic models of fuel cell components have been developed by Eikerling's group and Kulikovsky. These models are described in detail in the books written by Kulikovsky [18,19] and Eikerling [19]. Each of these models have varying levels of complexities and need for computationally simple models exist for easy implementation towards diagnostics and control in real time [20]. Model based diagnostics and rectification of PEMFCs has been reviewed by Petrone et al. [21].

Since fuel cells produce water as their product, it is essential to manage water appropriately to ensure its proper functioning. The fuel cell membrane requires hydration, while the GDL needs to be devoid of water. Removal of water from the membrane beyond a permissible limit leads to drying of the membrane, which results in a drop in ionic conductivity; whereas an excessive presence of water blocks the pores in GDL thereby restricting the reactant gases from reaching the electrode surface. This intricate balance in the water content that needs to be maintained during the operation of the fuel cell is called water management, and improper water management leads to performance loss. Several experimental studies on water balance are available in literature [22–24]. Fuel cell models dealing with water management issues in PEMFCs are of considerable importance due to their practical application potential. Various models handle water in the cathode side of the gas diffusion layer (GDL) in different ways to describe and quantify its influence on other cell operating parameters [25]. Fuller and Newman [26] considered water and thermal management simultaneously in a PEM fuel cell. Misran et al. [27] developed a steady state model considering the effect of operating conditions on water formation. Lee et al. [28] examined the effect of fabrication method, thickness of GDL, impregnation method of NAFION solution, and various other parameters on cell performance using numerical simulations. Yousfi-Steiner et al. [29] in their review on water management issues, explained two major conditions – drying and flooding, that results due to failure in water management. They also related the cause and effect of these states with the experimental parameters in a fault tree diagram, in addition to detailing the various characterization techniques and water management strategies.

To improve the durability of the fuel cell operation and for better water management, simple dynamic models are needed. Boaventura et al. [30] developed a dynamic 1-D model to describe the working of high temperature PEMFC (HT-PEMFC) considering water in gaseous state, which captured the transient behavior of the HT-PEMFCs. Similarly, developing a computationally efficient model to capture the unsteady state behavior of the PEMFC operating at low temperature accounting for water management is the major focus of our present work. As described before, while there has been considerable modeling effort in the literature, models that include liquid water, particularly in a dynamic fashion are relatively few. Further, such models tend to be rather complex, which will preclude their use in online control calculations. In this paper, we propose a simple dynamic first principles model that includes the effect of liquid water and its impact on the mass transfer resistance that develops in a low temperature fuel cell. This computationally efficient dynamic zero-dimensional model of PEMFC is validated with experimental data. We also describe the use of this model towards understanding the effects of water stalling and in the development of smart systems with a focus on water management.

Smart systems respond to changes in the operating conditions and environment, and trigger specific tasks to be executed based on stimuli received [31]. They can diagnose and activate a set of instructions to be carried out in order to protect the system under adverse conditions. Smart systems are becoming increasingly common in various electronics and consumer products. For successful implementation and operation of a fuel cell, smart systems that can diagnose and take corrective action towards getting the best performance from a fuel cell is necessary. Simple models can form an integral part of smart systems as they can be used to forecast the output from the fuel cell for implementation of appropriate remedial control actions.

Dynamic zero-dimensional model of PEMFC

A simple dynamic model accounting for transient behavior of low temperature PEM fuel cell has been developed in the present work. The schematic representing fuel cell cross-section considered in the development of the model is shown in Fig. 1. The anode feed is pure hydrogen and the