INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING, *SERIES B*
Volume 1, Number 2, Pages 123–146

A NUMERICAL MODEL OF THE CATHODE OF A PROTON EXCHANGE MEMBRANE FUEL CELL WITH EXPERIMENTAL VALIDATION

CHI-YUNG WEN, ANH DINH LE*, KUN-TSAN JENG, AND BIN-TSANG TSAI

Abstract. In this study, a simple two-dimensional, unsteady Proton Exchange Membrane Fuel Cell (PEMFC) model is developed and validated by experimental results. The numerical model considers fluid flow, mass transport and electrochemical reactions in the PEMFC cathode. The vorticity-stream function method and Alternating Direction Implicit (ADI) scheme are employed to solve the coupled fluid flow equations efficiently. The I-V characteristics obtained from the numerical model are in good agreement with the experimental results. The simulation results show that the gas flow velocity, concentration of oxygen and porosity of gas diffusion layer significantly influence the cell performance. Moreover, it could be inferred that, despite the real flow is three-dimensional, a two-dimensional numerical model is time-efficient to predict the location of liquid water formation and the fuel cell performance satisfactorily in some circumstances.

Key words. PEMFC, unsteady, cathode, vorticity-stream function, liquid water formation.

1. Introduction

The Proton Exchange Membrane Fuel Cell (PEMFC) is a kind of fuel cells that converts chemical energy from fuel and oxidant to electrical energy. Due to its environmentally-friendly characteristics of high efficiency, low emission/zero pollution and quite operation, the PEMFC is one of the most promising energy sources for use in automotive and portable electronics applications. A typical single PEMFC usually consists of an anode, a cathode and a polymer electrolyte membrane (PEM). Because the anode overpotential is negligible in comparison with the cathode overpotential[1], the coupled fluid flow, heat and mass transfer, and electrochemical processes at the cathode is much more significant than that at the anode. On the cathode side, oxygen is distributed to the electrode membrane region by the gas channel. Moreover, the gas channels play a major role in removing the by-product water from where it is generated. The gas diffusion layer (GDL) provides electrical contact between the electrode and the bipolar plate, distributes oxygen to the electrode, and allows product water to exit the electrode surface to the flow channel. Besides, the catalyst layer is added to speed up electrochemical reactions taking place on the electrode surface. Overall, the fuel cell processes involve the multi-component, multi-dimensional flow coupled with heat and mass transfer and electrochemical reactions processes. Due to these complex interactions, it is difficult to perform the experimental investigation to understand all the details of physics in a PEMFC during operation. Therefore, numerous numerical models have been developed for fuel cell simulations in recent years. One of the early one-dimensional mathematical models was presented by Bernardi and Vebrugge[2] in the beginning of 1990s, which simulated the cathode electrode of a

Received by the editors March 9, 2010 and, in revised form, November 14, 2010.
2000 *Mathematics Subject Classification.* 76M20 76D05.
The authors would like to thank the National Science Council of the Republic of China, Taiwan, for financially supporting this research under Contract No. NSC-94-2212-E-006-110.

polymer-electrolyte fuel cell. It focuses on polarization characteristics, catalyst utilization and water transport. After that, there have been more and more studies on PEMFC modeling that include cell performance prediction, mass transfer characteristics, and water management. Nguyen and Yi[3] developed a two-dimensional, steady-state, mass and energy transport model along the channel and across the polymer membrane. The distributions of gas pressure and temperature, as well as the current density along the channel were obtained. Taking the existence of liquid water into account, Wang et al.[4] considered the phase change of water within the cathode electrode and gas channel. They developed a two-phase transport model to predict the liquid water formation and its effects on the performance of the PEMFC cathode. It was found that the water transport (liquid and vapor) is controlled by capillary action and molecular diffusion, together with the very small air velocity within the porous electrode. Besides, a two-phase model based on the multi-phase mixture concept was developed further by You and Liu[5] for both anode and cathode. It predicted the formation and distribution of two-phase flow in the GDL and the gas channel simultaneously. Birgersson and Vynnycky[6] presented a detailed two-dimensional model for gas flow in the PEMFC cathode, in which the highly non-linear problem coupled with velocity and concentration fields were solved by the asymptotic method. Recently, a steady and unsteady, water and thermal management approach, considering the effects in both the along-channel and cross-membrane directions with detailed thermo-electro-chemical models, was developed by Huang et al.[7] to conduct fast and reasonable engineering optimizations. This study aimed at the effects of stack pressure, temperature, open circuit voltage, and water vapor on the membrane conductivity and cell performance. One of the three-dimensional models was presented by Berning et al.[8]. The three dimensional nature of the distribution of flow velocities, species concentration, mass transfer rates, electric current and temperature were illustrated by this model. It provided detailed insight into water transport mechanisms and mass transport limitations. Moreover, one remarkable finding was shown in this paper, which is: the net drag coefficients for the flux of water through the membrane are different for different values of electro-kinetic permeability of the membrane and the current density. Natarajan and Nguyen[9] developed a model for the PEMFC cathode by treating the third dimension along the channel with a so-called pseudo-three-dimensional model. The results render qualitative insights into the distribution of liquid water in the GDL and its effect on the distribution of the reactant species. Commercial CFD software packages such as Fluent, Star-CD, CFX, CFD-ACE+ etc. are commonly used in the fuel cell researches nowadays. Dutta et al.[10] presented a three-dimensional, single phase simulation for a PEMFC with Fluent. The geometrical model includes the flow channels and the GDLs on both anode and cathode sides. The complete three dimensional fluid flow, mass transport and electrochemical equations were solved with a control volume based discretization of the computational domain to obtain the pressure and velocity distribution in the flow channels and GDLs. Another three-dimensional, single phase mathematical model was conducted by Um et al [11]. The electrochemical and gas transport processes excluding water transport phenomenon inside GDLs and flow channels were solved using Star-CD software with PISO algorithm, the pressure implicit splitting of operators. Later on, Wang and Wang[12] extended the study of Um et al.[11] by examining additional physics involved in the water transport. The objective of this study is to introduce a mathematical algorithm to solve fluid flow, mass transfer and electro-chemical reactions processes simultaneously occurring in the cathode