Commun. Comput. Phys. July 2009

Fast Numerical Simulation of Two-Phase Transport Model in the Cathode of a Polymer Electrolyte Fuel Cell

Pengtao Sun^{1,*}, Guangri Xue², Chaoyang Wang³ and Jinchao Xu^{2,4}

¹ Department of Mathematical Sciences, University of Nevada, Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89154, USA.

² Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA.

³ Departments of Mechanical Engineering and Materials Science and Engineering, Electrochemical Engine Center (ECEC), The Pennsylvania State University, University Park, PA 16802, USA.

⁴ Laboratory of Mathematics and Applied Mathematics, School of Mathematical Sciences, Peking University, Beijing 100871, China.

Received 12 December 2007; Accepted (in revised version) 5 July 2008

Available online 13 November 2008

Abstract. In this paper, we apply streamline-diffusion and *Galerkin*-least-squares finite element methods for 2D steady-state two-phase model in the cathode of polymer electrolyte fuel cell (PEFC) that contains a gas channel and a gas diffusion layer (GDL). This two-phase PEFC model is typically modeled by a modified *Navier-Stokes* equation for the mass and momentum, with Darcy's drag as an additional source term in momentum for flows through GDL, and a discontinuous and degenerate convection-diffusion equation for water concentration. Based on the mixed finite element method for the modified *Navier-Stokes* equation and standard finite element method for water equation, we design streamline-diffusion and *Galerkin*-least-squares to overcome the dominant convection arising from the gas channel. Meanwhile, we employ *Kirchhoff* transformation to deal with the discontinuous and degenerate diffusivity in water concentration. Numerical experiments demonstrate that our finite element methods, together with these numerical techniques, are able to get accurate physical solutions with fast convergence.

AMS subject classifications: 65B99, 65K05, 65K10, 65N12, 65N22, 65N30, 65N55, 65Z05

Key words: Two-phase model, polymer electrolyte fuel cell, *Kirchhoff* transformation, convection dominated diffusion problem, streamline diffusion, *Galerkin*-least-squares.

*Corresponding author. *Email addresses:* pengtao.sun@unlv.edu (P. Sun), xue@math.psu.edu (G. Xue), cxw31@psu.edu (C. Wang), xu@math.psu.edu (J. Xu)

http://www.global-sci.com/

©2009 Global-Science Press

1 Introduction

Owing to their high energy efficiency, low pollution, and low noise, fuel cells are widely regarded as 21st century energy-conversion devices for mobile, stationary, and portable power. Through tremendous progress made in the past decade, currently available fuel cell materials appear to be adequate for near term markets with highest cost entry points. As a result, industries are currently placing their focus on fuel cell design and engineering for better performance, improved durability, cost reduction, and better cold-start characteristics. This new focus has led to an urgent need for identification, understanding, prediction, control, and optimization of various transport and electrochemical processes that occur on disparate length scales in fuel cells.

A fundamental fuel cell model consists of five principles of conservation [29]: mass, momentum, species, charge, and thermal energy. These transport equations are then coupled with electrochemical processes through source terms to describe reaction kinetics and electro-osmotic drag in the polymer electrolyte fuel cells (PEFC). Typically the fuel cell to be modeled is schematically shown in Fig. 1 and divided into seven subregions: the anode gas channel, anode gas diffusion layer (GDL), anode catalyst layer, ionomeric membrane, cathode catalyst layer, cathode gas diffusion layer (GDL), and cathode gas channel.

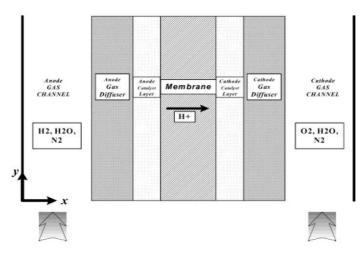


Figure 1: Schematic diagram of a polymer electrolyte fuel cell.

In this paper we specifically focus our interests on mass, momentum conservation and water concentration arising in gas channel and GDL of the cathode of PEFC. Highcurrent-density operation of PEFCs, is prone to liquid water formation due to excessive water generation at the cathode, resulting in two-phase transport phenomena. The transport processes then become significantly more complicated due to the coupled flow of liquid water and gaseous reactants in porous media. Moreover, the ensuing two-phase transport of reactant and product species becomes a limiting mechanism for cell perfor-