Journal of Computational and Applied Mathematics 270 (2014) 198–210

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Finite element approximation analysis for a steady state two-phase transport model of proton exchange membrane fuel cell

Yuzhou Sun *, Pengtao Sun

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

ARTICLE INFO

Article history:
Received 30 September 2013
Received in revised form 26 January 2014

Keywords:
Steady state two-phase transport model
Proton exchange membrane fuel cell (PEMFC)
Kirchhoff transformation
Finite element method
Optimal error estimates

ABSTRACT

In this paper, we study a 2D steady state two-phase transport model of water species which occurs in the cathode gas diffusion layer of proton exchange membrane fuel cell (PEMFC). The reformulation of water transport equation is described by Kirchhoff transformation to deal with the discontinuous and degenerate water diffusivity due to phase change. Finite element approximation is developed for the present model and the optimal error estimate in H^1 norm and the sub-optimal error estimate in L^2 norm are obtained for the multiphase mixture model of PEMFC for the first time. Numerical experiments are also performed to verify the theoretical results.

1. Introduction

Proton exchange membrane fuel cells (PEMFCs), owing to their high energy efficiency, low emission, and low noise, are widely considered as the most promising alternative power source in the 21st century for automotive, portable, and stationary applications. Fig. 1 schematically shows a single PEMFC. A typical PEMFC consists of several distinct components [1]: the membrane electrode assembly (MEA) comprised of a proton conducting electrolyte membrane sandwiched between two catalyst layers (CL), the porous gas diffusion layers (GDL), and the bipolar plates with embedded gas channels. In the anode CL, the hydrogen oxidation reaction (HOR) splits the hydrogen into electrons, which are transmitted via the external circuit, and protons, which migrate through the membrane and participate in the oxygen reduction reaction (ORR) in the cathode CL to recombine with oxygen and produce water and waste heat.

Water management is critical to achieve high performance of proton exchange membrane fuel cells (PEMFC), and is a significant technical challenge. Despite significant progress in recent years in enhancing the overall cell performance, a major limitation arises from the two-phase transport. This is primarily owing to the blockage of the open pore paths due to liquid water in the cathode gas diffusion layer, thus hindering oxygen transport to the active reaction sites in the catalyst layer. Gas diffusion layer plays a crucial role in the overall water management, which requires a delicate balance between reactant transport from the gas channels and water removal from the electrochemically active sites [2]. The polymer electrolyte membrane requires sufficient water to exhibit a high ionic conductivity. During fuel cell operation, water molecules migrate through the membrane under electro-osmotic drag, hydraulic permeation, and molecular diffusion, making it difficult to retain a high water content within the membrane. Generally, humidification is applied to the inlet gases of the anode and/or cathode in order to keep the membrane hydrated. On the other hand, water is generated in the cathode due to

* Corresponding author. Tel.: +1 7028859804.
E-mail addresses: suny5@unlv.nevada.edu (Y. Sun), pengtao.sun@unlv.edu (P. Sun).

http://dx.doi.org/10.1016/j.cam.2014.02.001
0377-0427/

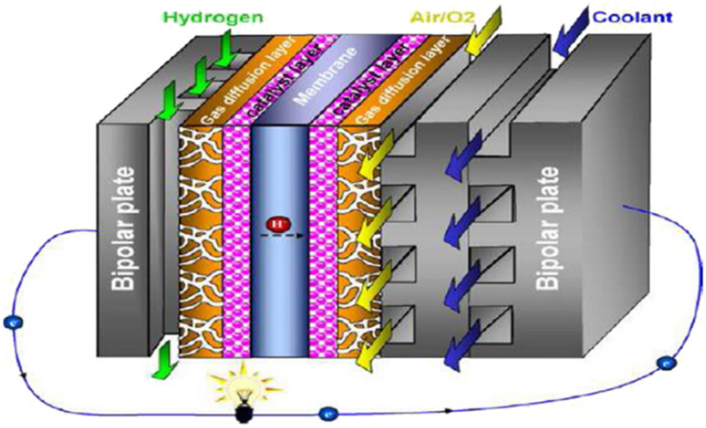

Fig. 1. A schematic 3D PEMFC.

the electrochemical reaction of H+/O2. If the water generated is not removed from the cathode at a sufficient rate, cathode flooding may result and the oxygen gas transport is hindered. Thus, a relatively dry air at the cathode inlet is sometimes helpful to remove excessive water [3]. Since there are two important and also conflicting needs in PEMFCs: to hydrate the polymer electrolyte and to avoid flooding in porous electrodes and GDL for reactant/product transport, in order to focus on the most important issue in PEMFCs—water management, only the water transport phenomenon, together with its two-phase transport modeling and its finite element approximation analysis are considered in this paper. The numerical analysis method carried out in this paper can be equivalently applied to other species transport equations occurring in FEMFCs.

For water concentration equation, in order to present a unified model that encompasses both the single- and two-phase regimes, and to ensure a smooth transition between the two, a discontinuous and degenerate function is introduced [4] as diffusivity of the transport equation in terms of water concentration. In gaseous water region, the water concentration is below a fixed value called saturated water concentration (16 mol/m^3 at 80 °C), coinciding with nonzero constant diffusivity. Once water concentration exceeds this fixed value, excess gaseous water is generated and condensed to liquid water. Correspondingly, water diffusivity suddenly jumps down to zero at this point and then slowly grows up to a smooth function with respect to liquid water concentration (a third degree polynomial in terms of liquid saturation). Thus a degenerate and discontinuous water transport equation is formed.

Compared to the numerous literature on modeling and experimental study of fuel cells, less work is contributed to the efficient numerical methodology of two-phase transport PEMFC model. Sun et al. [5,6,3,7,8] lead the field in numerical studies for PEMFC due to the cutting edge work on the efficient numerical techniques for the multiphase mixture (M^2) model of PEMFC, where, finite element method is adopted to discretize the governing equations of PEMFC model, and Kirchhoff transformation [9–11,6,7] is employed to specifically handle the derived discontinuous and degenerate water diffusivity arising in the two-phase water transport model of PEMFC with the intention to accelerate the nonlinear iteration and obtain an accurate solution. As for the corresponding theoretical analysis results, the error estimates of finite element method with Kirchhoff transformation was ever discussed for a simplified transient PEMFC model [12], however, not yet for the steady state PEMFC model. The goal of this paper is to accurately analyze the error estimates of finite element approximation for a simplified steady state two-phase transport model in the cathode gas diffusion layer (GDL) of PEMFC. We finally obtain the optimal error estimate in H^1 norm and the sub-optimal error estimate in L^2 norm for the present finite element approximation scheme. Numerical experiments are carried out as well to demonstrate the consistency between the numerical convergence rate and the theoretical result.

The rest of this paper is organized as follows. A simplified 2D steady state two-phase transport model in the cathode GDL of PEMFC is studied in Section 2. Then, in the same section, Kirchhoff transformation is introduced to describe the reformulated water concentration equation, and its efficiency is demonstrated in dealing with the discontinuous and degenerate water diffusivity. In Section 3, the finite element scheme is described and its approximation theorem is proved. In Section 4, the numerical experiment is carried out, in which a series of numerical convergence tests are given to verify the error estimate results proved in Section 3.

2. A simplified two-phase transport model in the cathode GDL of PEMFC

2.1. Model description

In this section, the governing equations for a simplified steady state two-phase transport problem in the cathode GDL of PEMFC, together with the computational domain and boundary conditions are described.