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Numerical Study of a 3D Two-Phase PEM Fuel Cell Model Via a Novel Automated Finite Element/Finite Volume Program Generator

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Abstract. Numerical methods of a 3D multiphysics, two-phase transport model of proton exchange membrane fuel cell (PEMFC) is studied in this paper. Due to the coexistence of multiphase regions, the standard finite element/finite volume method may fail to obtain a convergent nonlinear iteration for a two-phase transport model of PEMFC [49, 50]. By introducing Kirchhoff transformation technique and a combined finite element-upwind finite volume approach, we efficiently achieve a fast convergence and reasonable solutions for this multiphase, multiphysics PEMFC model. Numerical implementation is done by using a novel automated finite element/finite volume program generator (FEPG). By virtue of a high-level algorithm description language (script), component programming and human intelligence technologies, FEPG can quickly generate finite element/finite volume source code for PEMFC simulation. Thus, one can focus on the efficient algorithm research without being distracted by the tedious computer programming on finite element/finite volume methods. Numerical success confirms that FEPG is an efficient tool for both algorithm research and software development of a 3D, multiphysics PEMFC model with multicomponent and multiphase mechanism.

AMS subject classifications: 65B99, 65K05, 65K10, 65N08, 65N12, 65N22, 65N30, 65Z05

Key words: Proton exchange membrane fuel cell, two-phase transport, Kirchhoff transformation, finite element, finite volume, automated program generator, algorithm description language, script.

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1 Introduction

Fuel cells have been called the key to abundant energy from secure and renewable sources, e.g., fuel cells promise to replace the internal combustion engine in transportation due to their higher energy efficiency and zero or ultralow emissions. Hydrogen proton exchange membrane fuel cell (PEMFC) is presently considered as a potential type of fuel cells for such application. Since PEMFC simultaneously involves electrochemical reactions, current distribution, two-phase flow transport and heat transfer, an extensive mathematical modeling of multiphysics system combining with the advanced numerical techniques shall make a significant impact in gaining a fundamental understanding of the interacting electrochemical and transport phenomena and providing a computer-aided tool for design and optimization of future fuel cell engines.

Modeling and numerical simulation of hydrogen PEMFC have been attempted by a number of groups with the common goal of better understanding and hence optimizing fuel cell systems. Excellent reviews of hydrogen PEMFC research up to the mid-1990s were presented in [15, 39]. Recently, a comprehensive review of fuel cell science and technology was given in [60] which summarized the fundamental models for fuel cell engineering including single-phase and multiphase models. Single-phase model is the simplest approach in which the gas and liquid are considered as a single-fluid mixture and thus share the same velocity field. This approach is suited for fuel cell simulations under low humidity operation. The more rigorous approach to liquid water transport is a true multiphase model in which the two phases travel at different velocities. However, multiphase transport in fuel cells is always a challenge in fuel cell modeling. Multiphase flow, which especially exists at high-humidity operations, originates from water production by the oxygen reduction reaction, and the produced liquid water affects gaseous reactant supply and electrochemical catalyst activity as well.

There are two types of multiphase model existing for PEMFC modeling: multifluid approach and multiphase mixture (M^2) formation [61]. In contrast to those drawbacks of multifluid model [30]: a relatively large number of primary variables for each phase, highly nonlinear equations, numerical complexity due to explicitly track the irregular and moving interface between two phases, the M^2 model is more suitable for two-phase PEMFC modeling. One major advantage of the M^2 model over the classical multifluid model is that it eliminates the need for tracking phase interfaces, thus simplifying the numerical complexity of two-phase flow and transport modeling. Moreover, the M^2 model is mathematically equivalent to multifluid models without invoking any additional approximations. Therefore, we adopt M^2 formation as the two-phase transport model of PEMFC in this paper.

Comparing to the relatively plentiful literature on modeling and experimental study of fuel cells, there are less study contributing to the numerical method of two-phase transport PEMFC model. in [67], the volume-of-fluid (VOF) method is employed for PEMFC in conjunction with an interface reconstruction algorithm to track the dynamics of the deforming water droplets. However, VOF technique particularly deals with the interface