A Non-isothermal Modeling of a Polymer Electrolyte Membrane Fuel Cell

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Introduction

Polymer electrolyte membrane (PEM) fuel cells have attracted attention as an alternative power source in various applications such as vehicles, portable supplies, and stationary power systems. Although PEM fuel cells have been expected to be extensively used as an alternative power source, there have been many technical challenges to the implementation of PEM fuel cells. One of the most important issues is water and heat management in a PEM fuel cell stack. The control of water and heat is necessary for better performance and durability of PEM fuel cells.

The sufficient water content of the polymer membrane should be maintained to keep good proton conductivity, which is needed for better performance. In other words, the insufficiency of water on the anode side dries up the membrane, which deteriorates the performance. On the other hands, excessive water produced on the cathode side causes flooding to occur in the gas diffusion layer (GDL) and the gas channel (GC), which clogs pores and blocks the transport of oxygen to the catalyst layer (CL). This flooding results in the increase of voltage loss, causing reduced performance.

In a PEM fuel cell stack, heat is generated by the mechanisms, including irreversible heat, entropic heat, and Joule heating. Due to a large amount of heat generation caused by the electrochemical reaction, a peak temperature occurs at the cathode catalyst layer. The non-uniform temperature distribution has a significant influence on the water transport in PEM fuel cells. In addition, the hydration of polymer membrane strongly depends on different operating temperatures. The operating pressure as well as temperature critically influences thermodynamic states of water. Thus, it is important to understand the thermal behavior under different temperature and pressure conditions in order to maintain suitable water content and avoid the deterioration of membrane durability due to the formation of a hot spot.

The objective of the present work is to develop a 2-D non-isothermal PEM fuel cell model and investigate the non-uniform temperature effects on the performance under different operating conditions. The performance of a PEM fuel cell is optimized in terms of temperature, pressure, and water content.

Use of COMSOL Multiphysics

A non-isothermal PEM fuel model is developed and simulated by using Comsol Multiphysics. A PEM fuel cell modeling basically requires a multi-physics model which takes into account fluid flow, multi-species transport, current and electrical potential, and electrochemical reactions. Using Comsol Multiphysics, thermal modeling can be easily coupled with the electrochemical and mass transport models, allowing a comprehensive study of thermal and water behavior under various operating conditions.

The model is set up with conservation equations for charge, mass, momentum, species, and energy coupled with physical expressions using different application modes. Since charge transport is described by Ohmic's law, the Conductive Media DC application mode is used to calculate the potential distribution in a fuel cell stack. The Butler-Volmer equation which describes the reaction kinetics in the catalyst layers is used to determine current densities at both anode and cathode side.

Incompressible Navier-Stokes application mode and Darcy's law application mode are used to describe fluid flow in gas channels and porous media, respectively. Mass transport is mainly driven by the multi-component diffusion-convection so that the Maxwell-Stefan Diffusion and Convection application mode is adopted for species conservation in gas channels and porous media. Finally, the Conduction and Convection Heat Transfer module is incorporated to describe the thermal behavior in a PEM fuel cell stack. Temperature-dependent physical properties such as proton conductivity and diffusion coefficient are also included in Scalar Expressions to predict the temperature-dependent performance of a PEM fuel cell.