Numerical Simulation of Gas Flow with Electrochemical Reaction in a Polymer Electrolyte Fuel Cell

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Abstract

The aim of this dissertation was to investigate the performance of Polymer Electrolyte Fuel Cell (PEFC). The investigation involved understanding the mechanism of cross flow and pressure drop, addressing the contribution of cross flow on the performance, and water transport through the membrane. Computational fluid dynamics was used to study the gas flow behavior in the flow channel and porous media and information learned from the fluid dynamics study is used to design the artificial cross flow in the parallel flow field. At the beginning of the research, it was analyzed the mechanism of pressure drop and cross flow behavior in a single serpentine channel and gas diffusion layer. The dependency of physical parameters (e.g. porosity, permeability) and geometrical parameters such as gas channel pitch length and GDL thickness on the cross flow and pressure drop was studied vastly. It was explained pressure drop characteristics at the straight part of a serpentine channel and at the bend region. The role of cross flow on the pressure distribution in the gas channel also has been identified. Finally we concluded that the cross flow suppressed the pressure gradient in the straight part of serpentine channel and pressure gradient was maximum at the bend region. We also quantify the amount cross flow in terms of volume mass flux. The ratio of cross flow rate through the GDL to the total inlet flow rate increases with decreasing gas channel pitch length. Therefore, cross flow through the GDL can be enhanced by decreasing gas channel pitch length.

The aim of the second part of this work was to identify the contribution of cross flow on the performance individually. For this reason, a three dimensional single phase, isothermal model has been developed with considering the electrochemical reaction occurring in fuel cell. However, to avoid complicated two phase flow phenomena it was considered the constant hydration level in the membrane. The developed model was applied to an operating fuel cell to investigate the coupled flow, species transport and current density distribution. The gas channel pitch length effect on the performance has been evaluated by this developed model. The results show that it can capture all the physics occurring in PEM fuel cell very well. Because, it can capture the physics including activation overpotential, ohmic overpotential and mass transport overpotential very well. Hence, it proofs the applicability of our developed model. The gas channel pitch has marked effect on the performance of polymer electrolyte fuel cell. With decreasing of gas channel pitch it is found that the performance of fuel cell is increased. When cross flow was applied through the GDL and in between two channels of a parallel flow field, it was found that the performance of fuel cell increases in the mass transport region of polarization curve. The cross flow can enhance the oxygen transport towards catalyst layer. The simulation results show that the cross flow can help significantly to overcome the oxygen transport limitation; therefore, more electrochemical reaction occurs and result the performance improved. The convection flow caused by inlet flow rate also can increase the performance of PEFC. The effect of convection flow in current density is larger while using larger gas channel pitch length, whereas the thinner GDL has the larger convection flow effect in current density.

Finally we solve the water transport problem in the membrane of a PEM fuel cell which is one of the critical issues for PEFC performance improvement. Since, in the membrane water is transported from anode side to cathode side by electro osmotic drag flux caused by the proton transport. On the other hand, water is diffuse from cathode to anode side by back diffusion flux. Therefore, a delicate water balance is necessary to attain high proton conductivity of the membrane. In order to predict the water distribution in the different layer of PEFC, a three dimensional water transport model is developed which is able to capture the physics occurs in the membrane for transporting water from anode side to cathode side or vice-versa. To check the feasibility of our developed model validation test was carried out by comparing the simulation result with experimental work. This comparison validated the applicability of our developed model quantitatively for low relative humidity and qualitatively for higher relative humidity. The water content profile through the membrane was observed flat for relative humidity 40%. The water content profile in the membrane under the channel was lower than under the rib. With the increase of relative humidity the water content distribution through the membrane increases.

In this thesis, a complete single phase isothermal model has been developed to investigate coupled flow, species transport and electrochemical reaction occurring in PEFC. The cross flow has been analyzed vastly. The mechanism of cross flow and role of cross flow regarding pressure distribution in the gas channel, oxygen transport through the GDL, fuel cell performance improvement have been discussed in details. The water transport mechanism through the membrane also has been pointed out. Performance improvement of fuel cell has been clarified by a new design parameter cross flow.