Amirkabir Journal of Mechanical Engineering

Amirkabir J. Mech. Eng., 53(11) (2022) 1385-1388
DOI: 10.22060/mej.2021.19340.7004

Network Modeling to Investigate the Effect of Coupling the Transport Phenomena on Water Distribution in Gas Diffusion Layer

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ABSTRACT: The cathode side gas diffusion layer in polymer electrolyte membrane fuel cells discharges out the water generated as a result of the electrochemical reaction through its porous medium. This paper criticizes the generated pore network models for gas diffusion layers assuming uniform injection of liquid water from the catalyst layer. These models lead to a roughly uniform distribution of liquid water saturation in the in-plane direction making no difference between under gas channel and under rib regions which is in contradiction with the in-situ visualizations of gas diffusion layers. It has been attempted in this paper to couple the existing two-phase flow network models to other transport phenomena in the gas diffusion layer and also in other layers. To achieve this, the mentioned model is coupled to network models of oxygen and electron transport at the cathode side and also to a model of electrochemical reaction at the catalyst layer and a proton transport model of the membrane. As the first result of modeling, the distribution of local water generation rate and also the temporal evolution of total water generation rate at catalyst layer are presented, the latter experiencing an approximate 50% reduction from start-up to steady-state. The resulting water saturation distribution is strongly non-uniform, and maximums are observed under the ribs which is a direct result of non-uniform water generation at reaction sites.

Review History:

Received: Dec. 04, 2020
Revised: Jan. 29, 2021
Accepted: Feb. 25, 2021
Available Online: Mar.04, 2021

Keywords:

Pore network model
Gas diffusion layer
Polymer electrolyte membrane fuel cell
Two-phase flow
Coupling.

1- Introduction

1. Introduction

Polymer Electrolyte Membrane Fuel Cells (PEMFCs) are generally recognized as promising alternatives to internal combustion engines. One of the key challenges in PEMFCs is the water management issue which relies on a compromise between flooding of Gas Diffusion Layer (GDL) and dehydration of membrane both of which must be avoided. Cathode side GDL provides a passageway for reactant oxygen, electrons, and the generated water between Cathode Catalyst Layer (CCL) and Gas Channels (GCs) or the current collector ribs.

To simulate liquid water dynamics and two-phase flow in GDL, pore network modeling has proved as a valuable tool which has drawn attention in the last decade [1, 2]. The majority of the developed pore network models for GDL have assumed a uniform injection of liquid water from the catalyst layer into GDL, which is not actually what happens in the PEMFC electrodes. On the other hand, there have been few models in recent years taking advantage of coupled transport phenomena for a better representation of water dynamics in GDL [3, 4], however, the models merely integrate a predetermined water configuration in GDL to other phenomena while ignoring the liquid water invasion process.

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In this paper, a network model is proposed for GDL coupling the cathode side transport phenomena directly to the invasion process of water into GDL.

2- Methodology

At the first stage of modeling, a pore network is generated to adequately represent the pore space of real GDL in terms of porosity and permeability. The void space of GDL is represented by quadrilateral pores (ducts) and volumeless nodes. The pore sizes are distributed randomly according to a Weibull probability density function. To address the uncertainties accompanied by the statistical nature of network modeling, a large number of networks are generated and the results of the simulation are presented as averages and standard deviations of the results extracted from these networks.

At the second stage, two-phase water/airflow is simulated within the generated 2D networks. The capillary pressure model developed by Medici and Allen [1] is used. The volume flow rate in a pore is given by the modified Hagen-Poiseuille law as follows:

$$Q_{ij} = \begin{cases} \dfrac{{R_P}^2 A_w}{8\mu_{eff,ij} L}\left(P_i - P_j - P_{c,ij}\right) & , P_i - P_j > P_{c,ij} \\ 0 & , P_i - P_j < P_{c,ij} \end{cases} \quad (1)$$

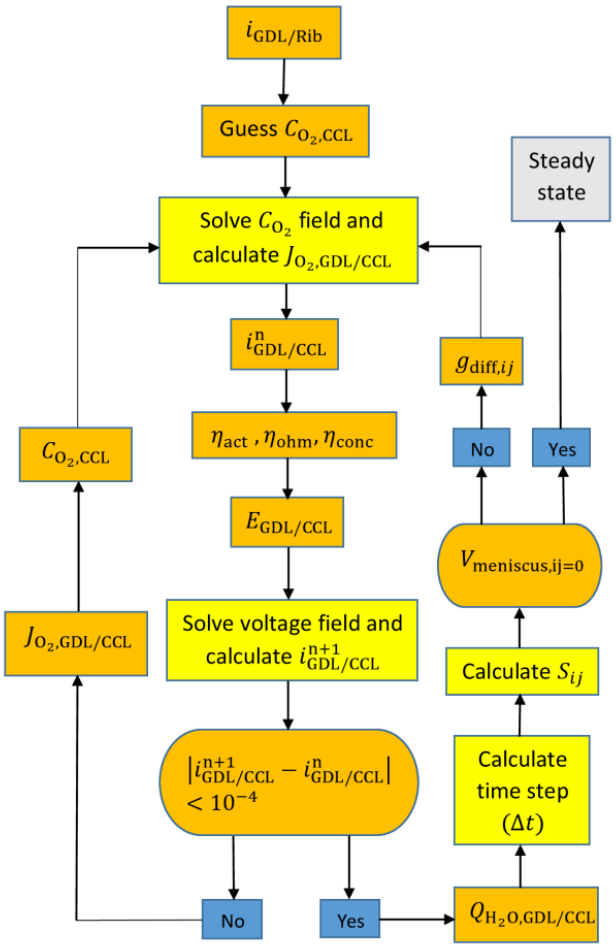

Fig. 1. Coupling algorithm of transport phenomena at the cathode side of the fuel cell

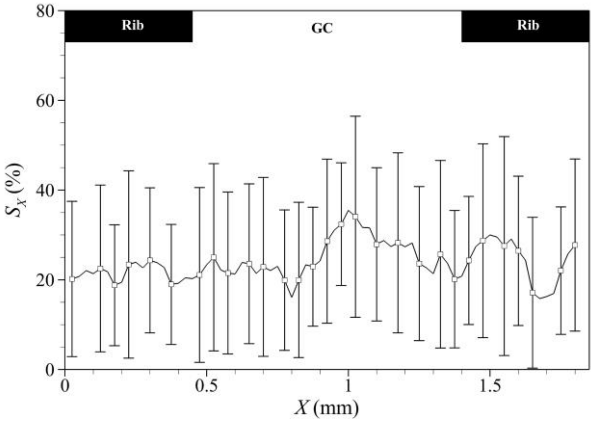

Fig. 2. In-plane saturation profile of liquid water in GDL

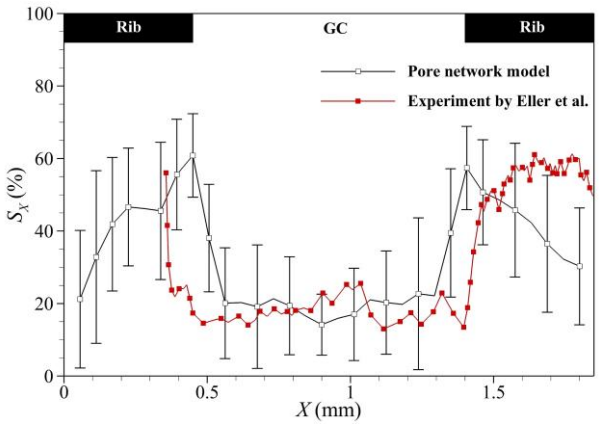

Fig. 3. In-plane saturation profile as a result of the coupled model. The saturation distribution of Eller et al. is also added for comparison [5].

where P_i and P_j are pressures at nodes i and j, $P_{c,ij}$ is the capillary pressure within pore ij, $\mu_{eff,ij}$ is the effective viscosity, R_p is the pore size, A_W is the cross-sectional area for water and L is the pore length. This part is carried out with the same assumption of uniform water injection from the catalyst layer as used in the mentioned references [1, 2].

At a third stage, first of all, the generated networks are upgraded to 3D, then it is attempted to couple the two-phase flow to other transport phenomena in the cathode side. To take the effects of oxygen and electron transport in GDL into account, network models are developed for them as well. The same void space in the generated networks is used for oxygen transport governed by Fick's law of diffusion. The solid walls of the pores are representative of carbon fibers of GDL and are assumed as pathways for electron conduction triggered by electric potential (E). A model of electrochemical reaction for catalyst layer governed by Butler-Volmer equation is used which leads to the determination of activation overvoltage (η_{act}). A proton transport model is used for the polymer membrane which results in the determination of ohmic overvoltage (η_{ohm}). Based on the drop in oxygen concentration (C_{O2}) in the catalyst layer, a theoretical relationship is used for the computation of concentration overvoltage (η_{conc}). The mentioned phenomena are coupled together according to the flowchart of Fig. 1, in which J represents mass flux, V is the meniscus velocity within a pore, and $g_{diff,ij}$ is the diffusive conductance of pore ij.

3- Results and Discussion

The simulations are carried out for a current density of i=0.75 A/cm2 and relative humidity of 100% in gas channels. As the main results of the model, saturation (S) distributions along the in-plane direction of GDL are produced. The non-coupled model which is based on the uniform injection of water as a boundary condition leads to the local saturation distribution depicted in Fig. 2. As spotted, the distribution is roughly uniform and no distinction can be spotted in the under the gas channel and under rib regions. This finding is in contradiction with the in-situ visualizations of GDL water distribution, however, similar models leading to similar results have been used before by the researchers [1, 2].

The in-plane saturation distribution as a result of the mentioned coupled model is portrayed in Fig. 3. As can be observed, water saturation is clearly higher under the

ribs as a result of non-uniform water generation in the catalyst layer which is now an output of the model. Also appended in Fig. 3 is the empirically determined saturation distribution of Eller et al. [5] which has been carried out for the same operating conditions as this paper. As can be seen, the agreement is satisfactory.

4- Conclusion

In the present research, it was attempted to improve the classic pore network models for GDL which had been predicated on the uniform injection of liquid water from the catalyst layer. To achieve this, the two-phase flow model was coupled to network models of oxygen and electron transport within GDL and also to an electrochemical reaction model of CCL and a proton transport model of the membrane. The model actually couples the local water generation rates as a result of the electrochemical reaction directly to the invasion process of water into GDL which renders it a transient model. As a main outcome of the model, water saturation was observed to have its maximum under the ribs while being minimum under gas channels which was in good agreement with experimental imaging of GDLs.

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HOW TO CITE THIS ARTICLE

H. Gholipour, M. J. Kermani , R. Zamanian, Network Modeling to Investigate the Effect of Coupling the Transport Phenomena on Water Distribution in Gas Diffusion Layer, Amirkabir J. Mech. Eng., 53(11) (2022) 1385-1388.

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