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3D Modeling of a fuel cell stack in COMSOL Multiphysics and design of humidity control system

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Abstract : Fuel cells are electrochemically reactive devices used extensively in transport, portable and stationary energy storage applications. The Proposed system is a multi-dimensional modeling of a stack of PEM fuel cells which are used in hybrid vehicles replacing batteries. Design of cell stack was done in CAD and stationary studies were done in COMSOL. The analytical model of the system is compared with the simulated results by including relevant physics in a PEMFC fuel cell operation. Simulation results were observed for variations in current density and electrolyte potential due to changes in operating conditions like humidity and temperature. Maximum current density was observed at 6.55e-4A/m^2. A novel design for automatic control of humidity within the membrane of fuel cell has also been proposed using ratio feedback.

Keywords : PEMFC, humidity, CNT, COMSOL™

1. INTRODUCTION

Proton exchange membrane fuel cells is one type of fuel cell, also known as polymer electrolyte membrane (PEM) fuel cells (PEMFC) developed for transport applications as well as for stationary and portable fuel cell power applications. PEMFCs comprise of membrane electrode assemblies (MEA) which include the electrodes, electrolyte, catalyst, and gas diffusion layers. In a PEMFC, the electrolyte used is a solid material compared to other fuel cells where the electrolyte is in liquid form. A single fuel cell can generate about 0.9-1.1V and so stack of fuel cells can be built to generate appreciable voltage. However the fuel cell performance degrades as the losses such as mass transport, activation, mechanical deformation and ohmic losses increases [14]. A fuel cell has the following sections: Gas diffusion layers, Backing layer, Catalyst, electrodes and an electrolyte1 as shown in Figure 1. The function of a GDL is to enhance the reactant gas flow through the membrane. The Backing layers are supporting layers made of thin carbon films which help in current conduction and effective water management. The Catalyst helps to speed up the reaction rate and in proton conduction. Platinum is widely used as catalyst. Anode and cathode electrodes are used for measuring the electrical output. The electrolyte is a micro porous membrane made of polymers, one such commonly used polymer is the Nafion. These composite membranes are on a great interest because of their temperature tolerance compared to other materials [13].

Literature review

From the works carried out earlier, it has been highlighted that performance of a fuel cell is greatly affected by moisture content of membrane [11]. A variation in current density for variation in electro osmotic flow has been reported for fuel cell with elliptical cross section [15]. Numerical simulation and stoichiometric calculations were

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performed by Lei Xing et al (2016) on PEMFC with varying heat transport indicated that cathode relative humidity was found to increase with decrease in anode humidity [16]. Daniel G.S eta al (2016) observed the voltage variations due to humidity variations at two different temperatures by considering a simple water balance model [17]. Choice of material has an invariable effect on fuel cell performance. CNTs as electrodes were found to have very high current density and proved to have good contact with the membrane [7].

2 MODELING AND SIMULATION

The fuel cell model is as shown in figure1. It consists of top and bottom plates, protecting the anode and cathode Gas diffusion layers, a catalyst layer and the proton exchange membrane. The model was simulated using Auto CAD^{TM} software and imported as the CAD model into COMSOL Multiphysics^{TM}. The dimensions of the model are given in the Table1. Materials for fuel cell and their properties were chosen from the Material library; the electrodes were chosen to be carbon nanotubes, GDL were chosen to be graphite and Polyimide as the membrane material.

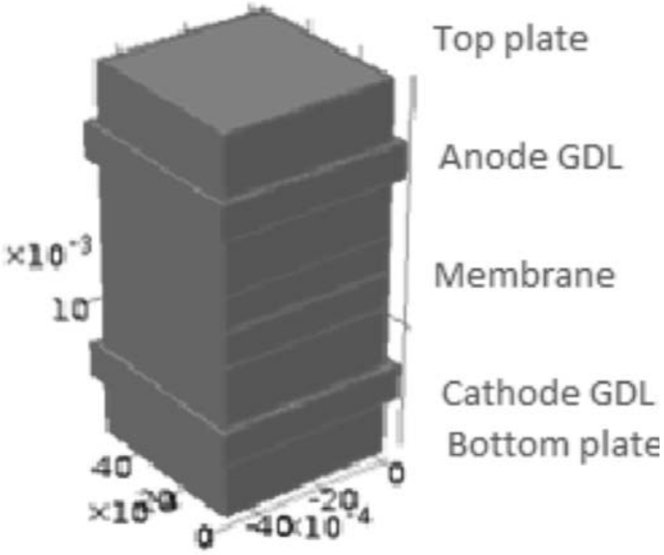

Fig. 1. A Fuel cell stack.

2.1. Meshing

The meshing was done by mapping. In total about 1364 edge elements and 40 vertex elements were studied. Minimum element size was found to be 3.6e-4m with the maximum element growth rate of 1.5. The model parameters for the above design are tabulated below.

Table 1. Model parameters

Parameter	*Value(m)*
Cell length	0.02
Channel height	1*e*-3
Channel width	0.78
Catalyst layer thickness	50*e*-3
Membrane thickness	100*e*-6
Electrode height	50*e*-6
GDL height	380*e*-6

2.2. Stationary studies

The following 2 physics were included in the model and stationary study was performed on the model – secondary current distribution (electric current) and solid mechanics. The cell operating condition was maintained at 120^o C, Pressure 1atm and Eigen frequency of 5.33Hz.

2.3.1. Secondary current distribution (siec)

Current distribution and the electro chemical characteristics of the cell can be studied by this physics. This gives an insight on how the electrical parameters vary with operating conditions.

2.3.2. Solid Mechanics

Since fuel cell operation involves redox reaction, heat flow occurs at the cathode layer in the form of steam byproduct. In order to determine the heat flux inside the device it is essential to add the heat transfer in solids physics to the fuel cell structure and by specifying the temperature and mode of operation, the heat distribution could be analyzed.

3. EXPERIMENT AND RESULT

The performance of a PEM fuel cell greatly depends on factors such as thickness of the electrode, thickness of the polymer membrane built and most importantly the moisture content present in the membrane. Since fuel cells generate electricity by giving water as a by-product, often the membrane of the fuel cell is exposed to water and over a period of time exposure to water vapor will degrade the membrane. During low humidity, the membrane becomes very dry and can brittle over longer cycles. On the other hand, during excess humidity, the membrane bloats and the ions can move without involving in the reaction. Thus an automatic control system is needed for maintaining optimum humidification inside the membrane. The figure 2 shows a novel design for sensing and regulating humidity using a ratio feedback control system.

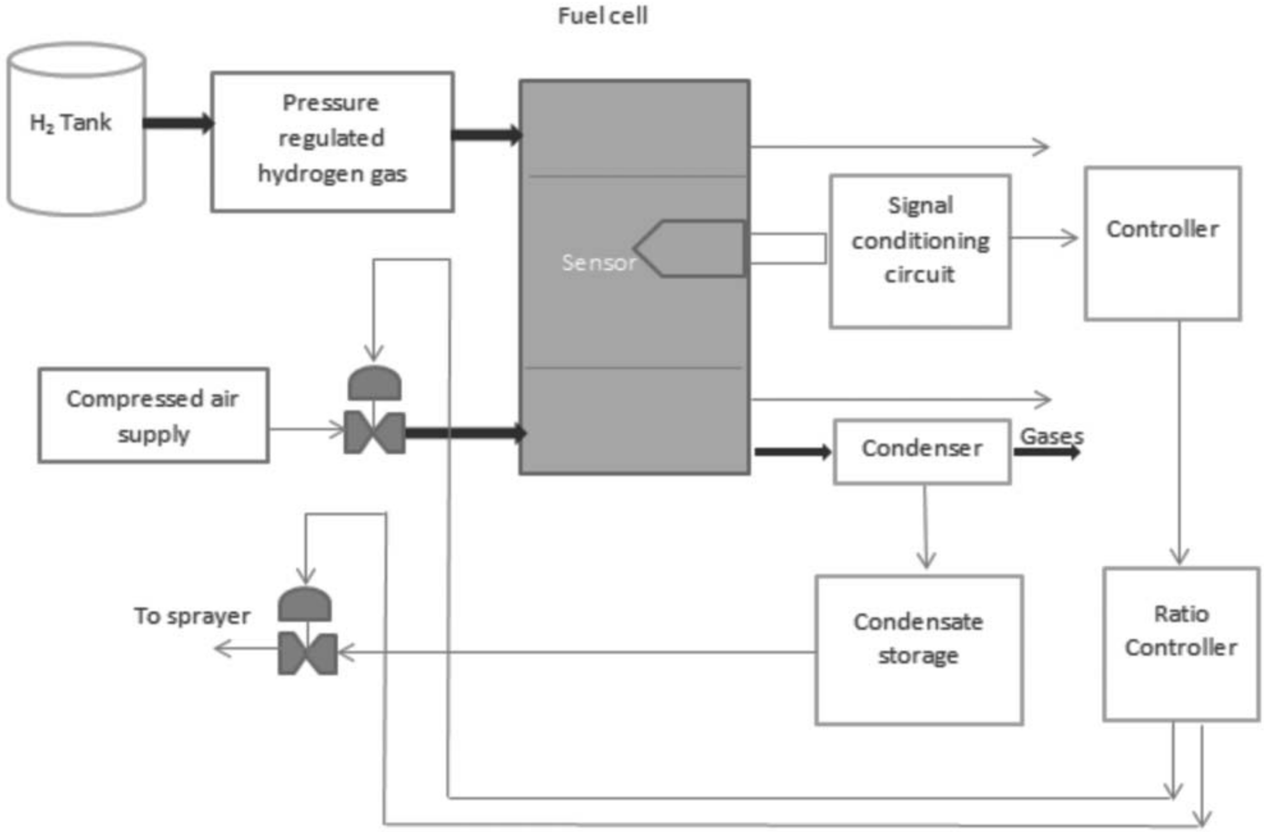

Fig. 2. Humidity control using ratio feedback

The proposed system has a mass flow controller for controlling flow of gases. At the anode and cathode sides pressure regulators are present in order to monitor the pressure of the gases. A thin film sensor of 1cm*1cm dimension is placed in the chamber of MEA with connecting leads and signal conditioned to get an appreciable output voltage. A ratio controller is fed with the set ratio and compares the actual ratio with the set point which is decided by a master controller. Any deviation in the ratio values is effected by adjusting the sprayer control valve % opening. Thus by this method humidity control can be achieved effectively.

Simulation Results

The following figures were obtained as a result of simulation. All the electrical parameters from membrane point of view are obtained as shown. Figure 3 shows a standardized electrolyte potential obtained at the membrane. Electrolyte potential was found to be uniform on either sides of the membrane for the forementioned operating conditions. Figure 4 shows the displacement, the membrane is subjected to due to the flow of the reactants during the electrochemical reactions. The displacement was estimated to be Maximum at the cathode side than the anode region which may be due to proton exchange towards the anode region. Figure 5 shows the current density produced at the membrane. The maximum value of membrane current density was observed to be 0.655mA/m^2.

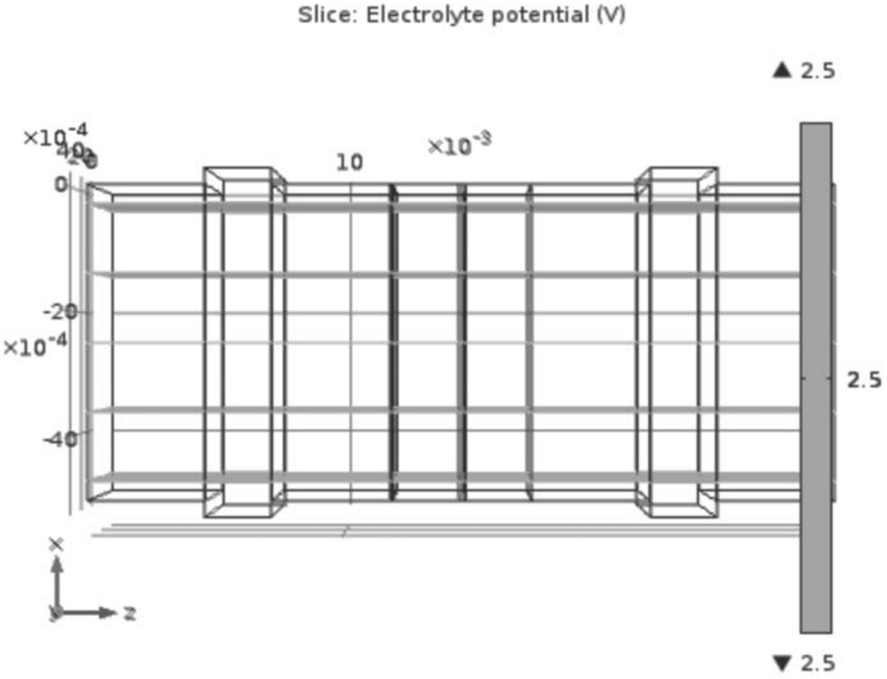

Fig. 3. Electrolyte potential

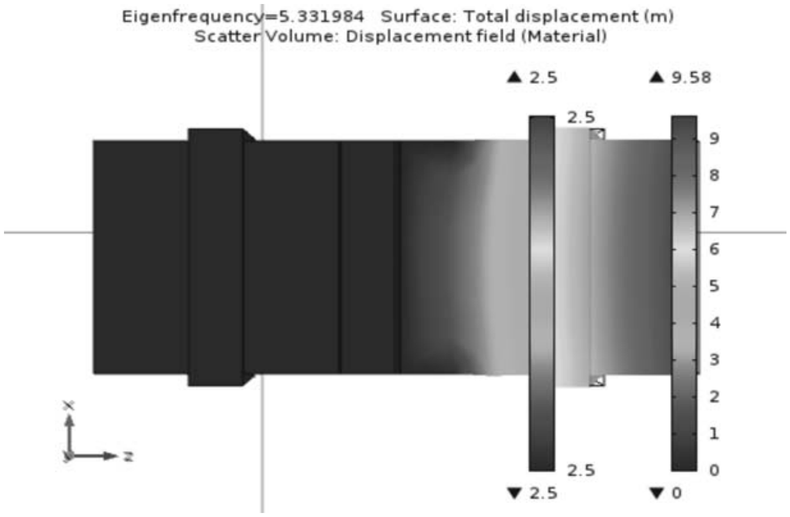

Fig. 4. Displacement of the membrane.

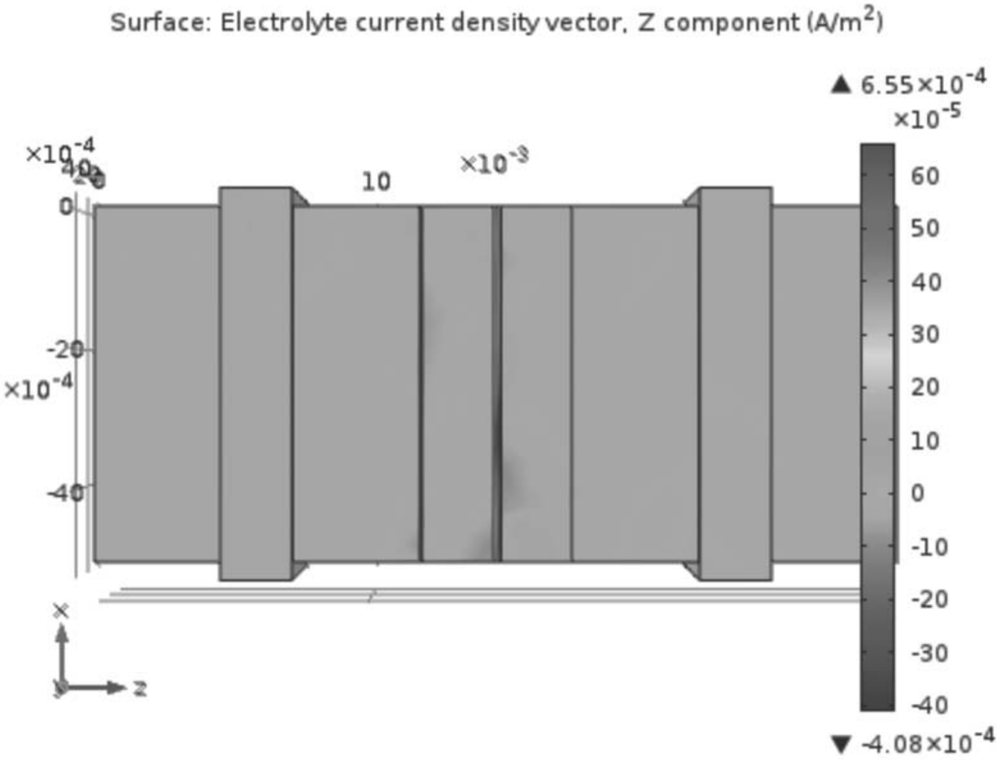

Fig. 5. Electrolyte membrane current density.

4. CONCLUSION

Thus the 3D model of a PEM fuel cell was simulated in COMSOL with relevant physics and the results indicated that the electrolyte current density varied from 4.08e-4A/m^2 to 6.55e-4A/m^2. The variation in current density is due to variation in the temperature contours inside the cell. As humidity and temperature are interdependent, the control of humidity can alter the cell temperature in turn the electrical output. By implementing the proposed automatic humidity control system, the membrane's exposure to water vapor could be studied and further an automatic method of removing the additional water from the membrane can be achieved for optimum humidification.

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