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Modelling of Gas Diffusion Layer of Polymer Electrolyte Membrane Fuel Cell: A Computational Approach

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In Polymer Electrolyte Membrane (PEM) Fuel Cell Gas Diffusion Layer (GDL) is the key component that makes electrical connection between the bipolar plates and the electrodes and helps in distribution of reactants to the electrocatalyst layers. Moreover, GDL allows the removal of produced water from the surface of the electrode and allow the motion of water in between the flow channels and two electrodes. It is well observed that the computational modelling plays an important role regarding the advancement in efficiency of PEM Fuel Cell. From the modelling perspective this is minutely examined that the GDL layer provides many objectives. Many approaches are being undertaken for the modelling of the GDL. Accurate prediction of the effective distribution of fuel, optimization of temperature and water management of GDL is important in understanding its effects on PEMFC performance. As the complex geometry is involved in GDL so the prediction of GDL behaviour is quite challenging. Hence, computational modelling of GDL is highly beneficial in this condition. This study aims to understand the influence of different parameters like temperature, Water vapor concentration, oxygen concentration, water vapour saturation on GDL performance. So, this work focuses on the study of the GDL computationally using MATLAB as the convenient programming language.

Keywords: Gas diffusion layer, Low temperature fuel cell, Computational modelling, Simulation.

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1. INTRODUCTION

In the Polymer Electrolyte Membrane (PEM) Fuel Cell, the outermost layer of the membrane electrode assembly (MEA) is GDL. Gas diffusion layer, catalyst and membrane layers are clubbed between the flow field plates. Different advantageous properties like mechanical support for the electrolytic membrane, electronic conductivity, provides porous layer to adhere and access of the reactants on the catalyst surface as well as product removal from GDL. This layer either consist of a single gas diffusion substance or composite structure and mainly carbon cloth or carbon paper is used in GDL. Fig. 1 illustrates a pictorial representation of the interior of the PEM fuel cell which depicts the motions in and outside of the GDL layer. Many approaches have been taken for the modelling of the GDL layer but this depends on how the other parts of the fuel cell is computationally modelled [1-3]. During electrochemical reactions at the electrode-electrolyte interface product water management is a great issue. So, for managing water, GDL allows only a specific amount of water to come in contact with the catalyst layer and electrodes so that Proton Exchange Membrane remains moisturized, whereas the rest of the water is eradicated. The wet proof layer is made as such that they can prevent the clogging of water molecules in the pores of carbon cloth or carbon paper which ensures the life span of Fuel Cell. The main purpose is to make gas diffusion layer hydrophobic to prevent any kind of flooding from product formation. The surface area of the porous media is important because the gaseous molecules diffuse into these porous media and makes better contact with a layer of a membrane electrode assembly (MEA). The water management and electrical properties get enhanced upon treatment of GDL with fluoropolymer and carbon black. These types of material found to encourage efficient spreading of reacting gases to membrane/electrode fabrication. The assembly of GDL permits fuel to disperse homogeneously on the catalyst surface which will help to increase the surface area of contact of catalyst layer membrane. There are ample number of literatures on porous media models, but there are less numbers of GDL models of fuel cells. As GDL model aims either on the corelation between solid support and the molecules or the flow through the support (the pores). Stefan-Maxwell equation regarding multicomponent gas diffusion and Fick's diffusion law regarding one component diffusion in a homogeneous medium can be employed when the focus was given on the modelling of the pores of the substrate. The implementation of kinetic theory on the interaction for both gas–gas and gas–solid molecules with the porous layer served like "dust" helps in deriving gas-solid interaction (known as Dusty Gas Model). Additionally, these models regard both the fluids, gas and liquid phases, or either of one. There exist majorly three types of GDL models such as Gas phase, Liquid phase and two-phase models. Models of Gas phase and Liquid phase presume that there exists only the motion of gas phase and the motion of liquid phase in the GDL, respectively. The gas-liquid interaction in a porous medium can be expressed by the Flow Models of the Two-phase. Besides the fluid transportation, the evaporation or condensation of fluids and electronic conduction of GDL are also the major properties of the layer. For Diffusion (Continuum) process different substance move to each other under the impact of oxygen concentration fed in the cathode layer, temperature, Water vapor concentration. Water vapor saturation. Although many modelling approach has been studied for different component of PEMFC [4-11]. These are the hydrogeological models that are derived from hydrogeological literature which are very useful. But there are some disadvantages due to the parameters like temperature, pressure, two phases, water vapour saturation, oxygen concentration etc are unknown [12-14]. In this paper, we have done the modelling of the GDL incorporating the influence of several factors for both the electrodes.

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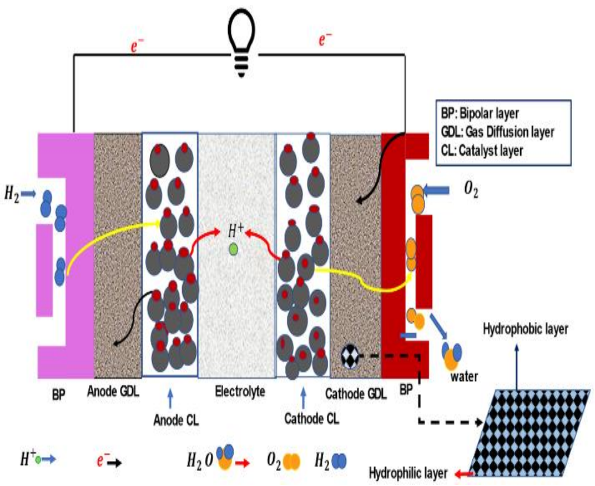

Fig. 1 – Schematic of flow of fuel through the GDL for PEMFC

2. METHOD OF COMPUTATIONAL MODELLING

For modelling of the GDL for the PEMFC, MATLAB software (2022), Windows 10 is used. The equations and the same methodology for computational modelling of the GDL developed by Beuscher et al. [15] were used.

3. RESULT AND DISCUSSION

All the plots generated by MATLAB come with a scale ranging from lowest value to highest value and helps to explain the relationship. As the fuels keep on entering the layers of GDL, there is a rise in temperature which is depicted using the temperature contour plots (Fig. 2) in YX plane.

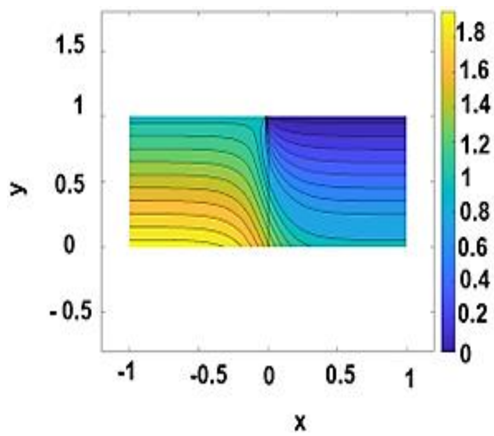

Fig. 2 – Contour plot of temperature

The grid point numbers in the x and y direction are considered to show the variations. It is relevant to mention here that in the figure, when the boundary conditions are examined by keeping pressure constant, the regions are symmetric about $x = 0$ in both positive and negative x axes. In order to compute the interrupt domain, 2D finite difference methods are used. Same plot for the distributions of water vapour in XY plane is obtained at Fig. 3.

In the case of fuels, we know that hydrogen and oxygen react to form water vapour and MATLAB programming is done in this case too, which shows that concentration of water vapour gradually increases. The same thing is reflected in Fig. 4.

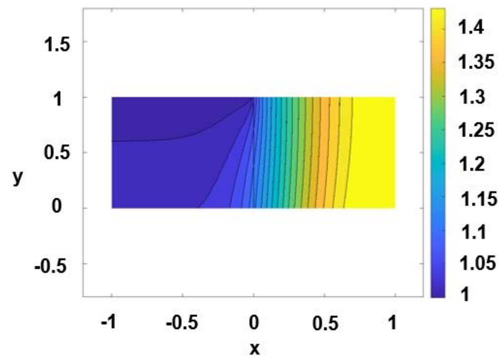

Fig. 3 – Water vapor concentration

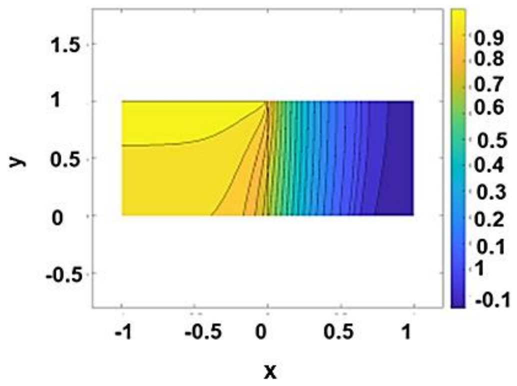

Fig. 4 – Water vapour saturation

More the reaction, more will be the product formation. In addition to these two plots, 2D plots which is done using MATLAB for the oxygen concentration is depicted in Fig. 5. The scales are same as Fig. 2 here. It is proved that the derivation of oxygen concentration is similar to the derivation of temperature.

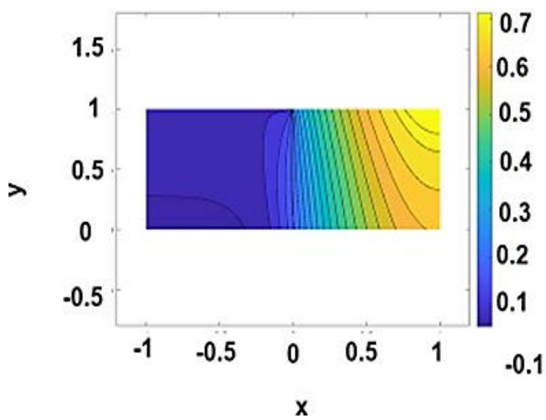

Fig. 5 – Oxygen concentration

The GDL layers are two dimensional and hence the XY plane in the plots depict the correlations in Fig. 2, 3, 4, 5 only. In all of the Fig. 2-5, it is evident that as expected form the theoretical aspect, all the distributions are symmetry with respect to Y-axis. A 3D plot using MATLAB to get the temperature of inner surface by utilizing the derived equations. The temperature plot in the interior surface is exhibited in Fig. 6. These MATLAB code generated plots relate to the Gas diffusion layer. They correspond to the concentration and saturation levels of by-products formed and also the reactant gases that are fed.

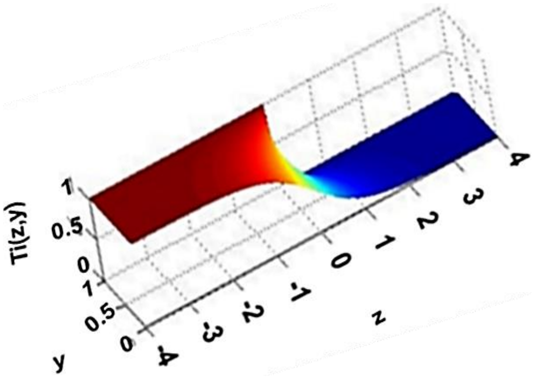

Fig. 6 – 3D PLOT of temperature

4. CONCLUSION

From the above discussed modelling, we can conclude that across the GDL, thermal distribution is driven by the boundary conditions of temperature. GDL also has the capacity for water management. MATLAB is a useful tool for the computational modelling of GDL.

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Моделювання газодифузійного шару паливного елемента з полімерної електролітної мембрани: обчислювальний підхід

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У полімерно-електролітній мембрані (PEM) газодифузійний шар паливного елемента (GDL) є ключовим компонентом, який забезпечує електричний зв'язок між біполярними пластинами та електродами, а також допомагає розподіляти реагенти до шарів електрокаталізатора. Крім того, GDL дозволяє видаляти вироблену воду з поверхні електрода та допускати рух води між проточними каналами і двома електродами. Відомо, що обчислювальне моделювання відіграє важливу роль у підвищенні ефективності паливних елементів PEM. Багато підходів використовуються для моделювання GDL. Точне передбачення ефективного розподілу палива, оптимізації температури та управління водою GDL є важливим для розуміння його впливу на продуктивність PEMFC. Оскільки в GDL бере участь складна геометрія, прогнозування поведінки GDL є досить складним завданням. Це дослідження має на меті зрозуміти вплив різних параметрів, таких як температура, концентрація водяної пари, концентрація кисню, насичення водяною парою, на продуктивність GDL. Таким чином, дана стаття зосереджена на вивченні GDL з використанням MATLAB як зручної мови програмування.

Ключові слова: Політерно-електролітна мембрана, Газодифузійний шар, Низькотемпературний паливний елемент, Обчислювальне моделювання.