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Mass Transport Analysis of a PEM Fuel Cell (High Temperature-PEMFC) Under Different Operating Conditions

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Abstract: Fuel cells are devices which convert the chemical energy in the fuels into electrical energy through electrochemical reactions PEM fuel cells use a solid polymer as a membrane with graphite electrodes.The problem with Platinum catalysts is that even though they speed up the reaction rate, they are attractive towards toxic gases. Proposed system is a multidimensional modelling of PEM fuel cells. The analytical model of the system is incorporated with the simulated results obtained through various physics studies involved in a PEMFC fuel cell operation. The various operating conditions for the study include catalyst replacement, membrane replacement at different operating temperatures .Through these operating condition variations, the simulation result gives the mass transport of reactants and oxygen through the electrodes.

Index Terms: Polymer electrolyte membrane, catalyst, transport analysis

Acronyms used: –PEM-Polymer Electrolyte Membrane

1. INTRODUCTION

An eco-friendly electro-chemical device which converts the chemical energy in a fuel into electricity are referred to as a fuel cell. It is often denoted to as a green energy converting device since it is a no pollution power supplier. There are various types of fuel cells which take in different fuels and generate electricity and provide useful by-products. These fuel cells do not infest the air with harmful greenhouse gases.

A fuel cell has the following sections: Anode slot, Cathode slot each consisting of a Gas diffusion layer, Catalyst and an electrode .The two slots are located separated by a membrane which acts as an electrolyte.

The function of a GDL (Gas Diffusion Layer) is to enhance the reactant gas flow through the membrane. The catalyst helps to speed up the reaction rate and in proton conduction. Anode and cathode electrodes are used for measuring the electrical output. The electrolyte plays a key role in the functioning of a fuel cell; it can be of solid or liquid form. In case of PEMFC the electrolyte is a micro porous membrane made of polymers as shown in “Figure 1”.

These fuel cells are of portable type and can generate high current output even if they operate at low temperature (80^{o}C) but HT PEMFC are of better concern because with LT PEMFC, performance is greatly affected by water concentration in the membrane and the catalyst performance [6].

2. LITERATURE REVIEW

From the works carried out earlier, it is highlighted that, performance of a fuel cell is greatly dependent on the material chosen for the membrane and electrode [9]. VACNTs as electrodes were found to have very high current density and proven to have good contact with the membrane[8].Membrane materials must satisfy high temperature requirement and low humidity requirements. Hydrous materials such as Polyamides and Polysulphones are of great interest [13].

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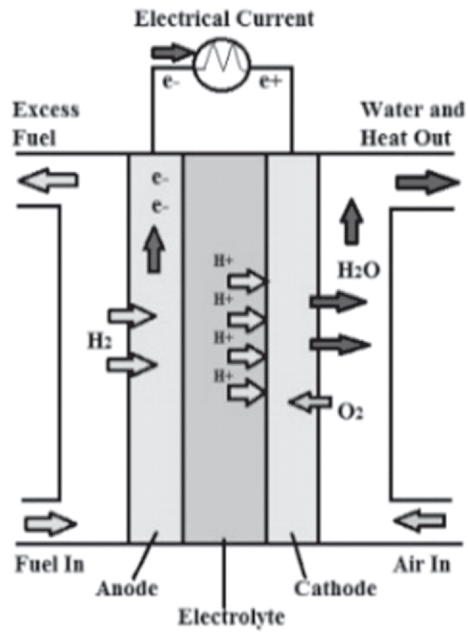

Figure 1: PEM Fuel Cell

Also the performance of a fuel cell is highly temperature dependent. During low temperature, loading of platinum catalyst is pronounced, which is counteracted if operated at high temperatures [6].

3. FUNDAMENTALS OF FUEL CELLS

The basic fuel cell reaction is Hydrogen oxidation reaction at the anode and reduction reaction at the cathode. The electrons after the generation of electricity combine with hydrogen ions that pass through the membrane and oxygen at the cathode and give out water as by-product. The following "Eq. 1" and "Eq. 2" shows the redox reaction in the fuel cell

Anode: $$2H_2^- \rightarrow 4H^+ + 4e^- \quad (1)$$

Cathode: $$4H^+ + 4e^- + O_2^- \rightarrow 2H_2O \quad (2)$$

4. MODELLING SETUP

The structure consists of rebuilding of a HT PEM fuel cell as a straight channel. The structure consists of three slots namely the Anodic slot, Cathodic slot each consisting of electrodes, gas diffusion layer and a catalyst layer. Both the slots are sandwiched between a membrane which plays a vital role in generating a protonic potential in the fuel cell. Each part of the fuel cell are built as separate units.

5. MATERIALS

Proper understanding on the operation of a PEM fuel cell is essential to rightly specify the materials for each of the layers in the cell. Graphite electrodes that were used previously as electrode material [7], were replaced by carbon nanotubes [6].Reformate gas which is used as a fuel contains small amount of carbon monoxide (CO), which decimates the platinum catalyst affecting the steady operation of a PEMFC [6]. Thus replacing the catalyst with another material would avoid this shortcoming to an extent. Cobalt was chosen as a material of choice. Composite membranes are on a great interest so as to increase the temperature tolerance compared to other materials [3][7]. Polyamides are used as materials for membrane which has high thermal conductivity. Graphite plates are used as gas diffusion layer material.

6. MODEL DEFINITION

A PEMFC model shown has been virtualized. The study was initially started with the conventional electrode and GDL and later changed to the proposed CNT and graphite [5]. The structure developed is shown in "Figure 2".

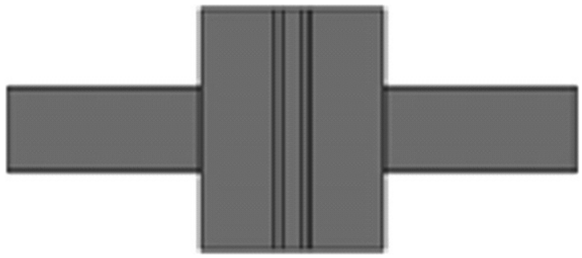

Figure 2: 2D view of simulated model of a PEM

7. OPERATING CONDITIONS

The analysis was performed at higher temperatures, chosen temperature was 120°C, 80°C and the results were obtained for the fluid flow in a fuel cell considering cobalt as a catalyst. A reference concentration of the reactants was given as 40.88 mol/m^3. The cell was operated at absolute pressure conditions. The structure was mapped completely and swept with specific sizing specifications.

8. RESULTS AND DISCUSSIONS

Accordingly, a straight channel structure of the fuel cell was applied with the required boundary conditions and was subjected to the different physics to properly define the operational principle of this device. The cell was operated at a pressure of 101 KPa. The structure was mapped completely and swept with specific meshing size. The amount of hydrogenand water present in the cell were analyzed using cobalt as a catalyst. "Figure 3" shows the hydrogen concentration, "Figure 4" shows the water concentration at a temperature of 120 degrees and "Figure 5"and "Figure 6" shows the hydrogen and water concentration in a single fuel cell. Fluid transport analysis at 80 degrees, 120 degrees using cobalt as catalyst is shown below.

TEMPERATURE: 120°C

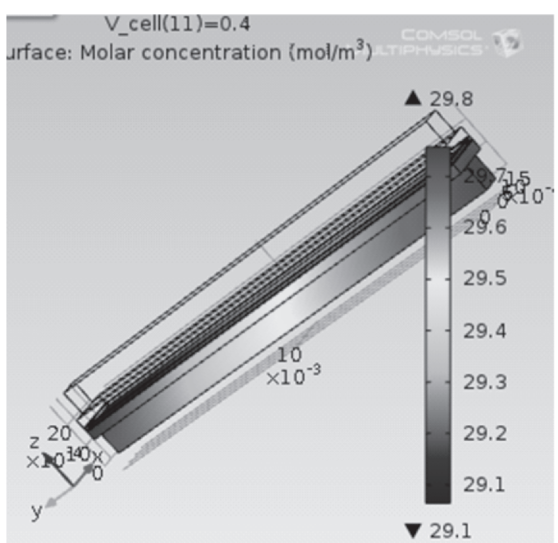

Figure 3: Anode Hydrogen Concentration at the cathode using cobalt at temperature of 120°C. Simulations were run absolute pressure with a reference concentration of 40.88 mol/m^3

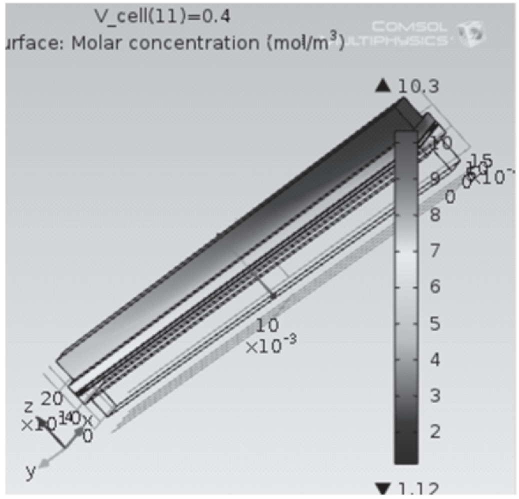

Figure 4: Water concentration present at the cathode slot for a reference concentration of hydrogen and oxygen as 40.88 mol/m^3

TEMPERATURE: 80^{o}C

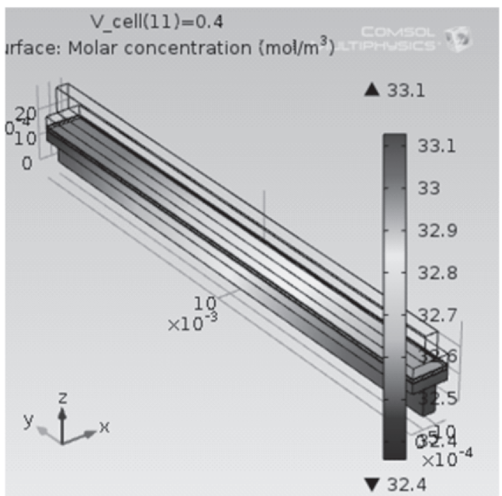

Figure 5: Anode Hydrogen Concentration at the cathode using platinum at temperature of 80°C. Simulations were run absolute pressure with a reference concentration of 40.88 mol/m^3

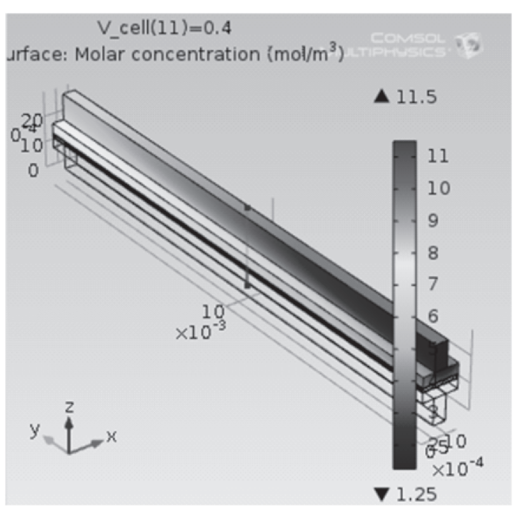

Figure 6: Water Concentration along the cathodic slot of the fuel cell for a reference concentration of 40.88 mol/m^3

9. INFERENCE AND PROSPECT

As the temperature of operating the fuel cell increases, so does the requirement of removing the water present in the cathode reduces. It is seen that using cobalt, the water concentration is quite less in the range of 2-9.84 mol/m^3. But with using platinum there are chances of formation of carbon monoxide as per literature. Platinum being a noble catalyst is expensive. So it is possible to replace this with cobalt without affecting the fuel cells performance. Moreover it is understood that by determining the transport of fluid through the fuel cell modelling, further optimization on the device performance could be done. However work is continued to concentrate only on the membrane of a fuel cell in order to enhance the performance of fuel cell by monitoring the amount of exposure to water vapour.

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