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MODELING AND FINITE ELEMENT MASS TRANSPORT ANALYSIS OF A POLYMER ELECTROLYTE MEMBRANE FUEL CELL AT DIFFERENT OPERATING CONDITIONS

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ABSTRACT

In this investigation, a 3-D modeling of a PEM (polymer electrolyte membrane) fuel cell has been presented by considering Carbon nanotube (CNT) as the electrode and Cobalt as catalyst. Conventional fuel cells utilize graphite electrodes and platinum catalyst. Compared to mechanical and electrical properties of graphite, CNTs offer good mechanical strength and high current density. Similarly Cobalt has been considered as a cost effective counterpart to platinum. The simulation was carried out at 3 different operating temperatures (80°C, 120°Cand 160°C) and the results were analyzed. The focus of this work is to design, analyze and compare the water concentration at the cathode side, using the above two catalysts.

Keywords: polymer electrolyte membrane fuel cell (PEMFC), GDL, CNT, modelling, catalyst, COMSOL™.

Acronyms used

PEM Polymer Electrolyte Membrane
LT Low Temperature
HT High Temperature
GDL Gas Diffusion Layer
CNT Carbon Nanotubes

INTRODUCTION

A fuel cell is a **green** electro-chemical device which converts the chemical energy of a fuel into electrical energy. The term **green** arises since it is a non-polluting power generator. There are several types of fuel cells which take in different fuels and generate electricity and give out useful by-products. For instance, from a Hydrogen fuel cell, we get a useful by-product water along with electrical output. A stack of such fuel cells can be combined to generate appreciable voltage. These fuels do not pollute the atmosphere with harmful greenhouse gases. A fuel cell has the following sections: Anode compartment, Cathode compartments each consisting of a Gas diffusion layer, Catalyst and an electrode. The two compartments 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.

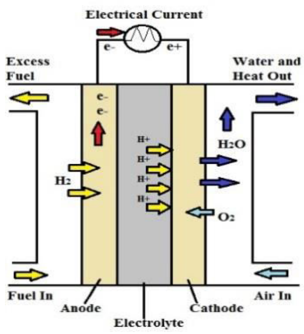

Figure-1. PEM Fuel Cell.

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]. CNTs as electrodes were found to have very high current density and prove to have good contact with the membrane [8]. Reformate gas which is used as a fuel contains small amount of carbon monoxide (CO), which exterminates the platinum catalyst affecting the regular operation of a PEMFC [6]. Membrane materials must satisfy high temperature requirement and low humidity requirements. Hydrous materials such as polyamides and polysulphones are of great interest [13]. 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]. Motivated by these observations,

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the following work, analyzes the transport mechanism at three different temperatures using a cost effective catalyst.

FUNDAMENTAL LAWS ASSOCIATED WITH 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.

Anode: $2H_2 \longrightarrow 4H^+ + 4e^-$
Cathode: $4H^+ + 4e^- + O_2 \longrightarrow 2H_2O$

Darcy's law

The Darcy's law relates the velocity and viscosity of a fluid when it flows through a porous/permeable structure having small sized pores. It is given by

$$\frac{\partial \rho}{\partial t} + \nabla . \rho \mu = 0$$

Where
ρ: Density of the fluid
μ: Dynamic viscosity

Brinkman's equation

Since Darcy's law deals with flow through micro pores and Stokes equation describes the flow through macro pores, pressure gradient at the boundary between the two regions is described by

P= $-\mu/K$*V+μ_e*μ_e*V
Where
μ_e: Effective viscosity in porous media
V: Velocity
K: Permeability of porous media

Tafel's equation

The hydrogen reaction rate directly determines the current density of a fuel cell. When the current density is higher, there is a drop in the potential called as over potential. This drop is due to the resistance to flow of current at higher current densities. The following equation describes the relation between the over potential and the current density.

$\Delta V = A * ln(I/Io)$
Where
A: Tafel's constant
I_o: Exchange current density (mA/cm^2)

MODELLING SETUP

The structure consists of a detailed 3D volume based rebuilding of a HT PEM fuel cell. The structure consists of three compartments namely the Anode and Cathode compartments each consisting of electrodes,

Gas Diffusion Layer (GDL) and a catalyst layer. The electrodes are chosen to be Carbon Nano Tubes (CNTs) and Catalyst is chosen to be Cobalt. Both the compartments are sandwiched on either side of a membrane which plays a vital role in generating a proton potential in the fuel cell. Each part of the fuel cell is built as separate block.

Assumptions

- The fluid used is incompressible.
- Pure oxygen is used at the cathode.
- The fuel cell operation is time-independent.
- Membrane is humidified completely.
- Flow is taken to be laminar.

MATERIALS

In order to have a proper understanding on the operation of a PEM fuel cell it is essential to rightly specify the materials for each of the layers in the cell. As the modeling involved was to optimize the design of a PEM fuel cell, to enhance the performance of it, choosing the best material was vital. Graphite Electrodes that were used previously as electrode material [7] were replaced by carbon nanotubes as they have really high strength and improved gas diffusivity, water drainage, and effective use of the catalyst [6]. Cobalt was chosen as a material of choice as it proved to be more stable than platinum and one of the major advantage is, it is of low-cost [12]. The material to be used for the membrane must be able to absorb some amount of the flowing reactants. Composite membranes are on a great interest due to their temperature tolerance compared to other materials [3].Polyamides are used as material for membrane which has high thermal conductivity. Graphite plates are used a gas diffusion layer material.

MODEL DEFINITION

A PEMFC model shown has been simulated using COMSOL Multiphysics^{TM}. The study was initially started with the conventional electrode and GDL and later changed to the proposed CNT and graphite. The following physics were included during simulation and the stationary study was done.

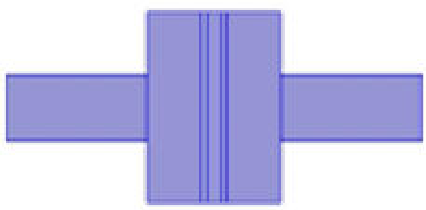

Figure-2. 2D view of simulated model of a PEM.

PHYSICS INVOLVED

Secondary current distribution

Application of this physics to the entire structure helps to study the electro kinetics in the fuel cell. This physics gives indication of voltages and currents generated in the system.

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Reacting flow through porous media-transport of concentrated species

The transport of concentrated species interface is used to study gaseous and liquid mixtures where the species concentrations are of the same order of magnitude and none of the species can be identified as a solvent. This physics interface includes models for multicomponent diffusion, where the diffusive driving force of each species depends on the mixture composition, temperature, and pressure. The physics interface solves for the mass fractions of all participating species.

Operating conditions

The analysis was performed at three different temperatures (80°C, 120°Cand 160°C). The results were obtained for the mass transport of a fuel cell considering platinum as a catalyst as well as cobalt. A reference concentration of the reactants was given as 40.88mol/m^3. The cell was operated at a pressure of 101KPa.The structure was mapped completely and swept with specific meshing size as shown in Figure-3. Stationary study was performed and the following results were obtained.

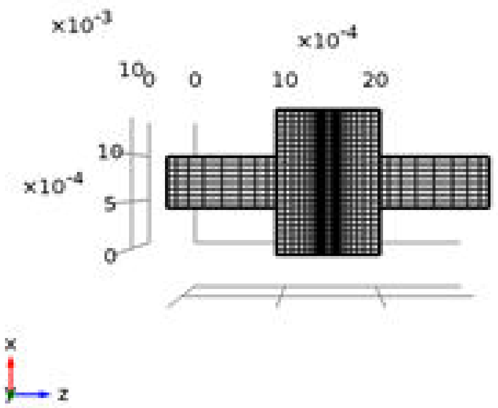

Figure-3. Structure after meshing.

RESULTS AND DISCUSSIONS

A single straight channel fuel cell operating at three different temperatures was studied with an operating cell voltage $V_{\_cell}$ of 0.4V. This study was performed to compare the variations inthe amount of water concentration at the cathode side by using different catalyst. It has been observed that when operated at high temperature, the water concentration tends to reduce. Simulations were carried out using both the catalyst at same operating conditions as shown below.

Figures 4 and 5 indicate the water concentration at a temperature of 160°C for the catalyst platinum and cobalt respectively. Figures 6 and 7 present the molar concentration of water at a temperature of 120°C. Similarly Figures 8 and 9 compare the cathode water accumulation at a temperature of 80°C.It has been found that optimal performance of the fuel cell is affected if there is excess water in its stack. Hence water management is imperative in ensuring proper functioning of fuel cell.

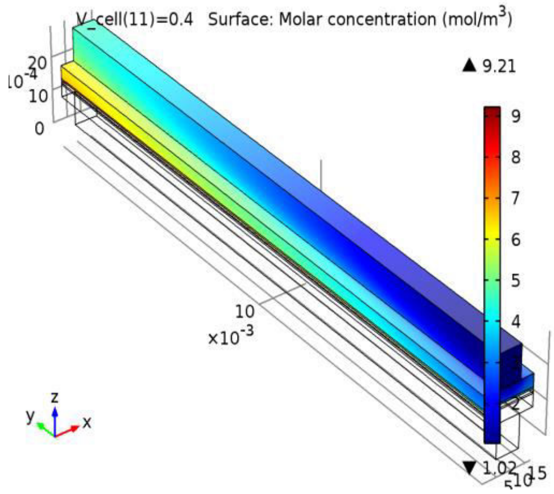

Figure-4. Water concentration at the cathode using platinum at temperature of 160°C.

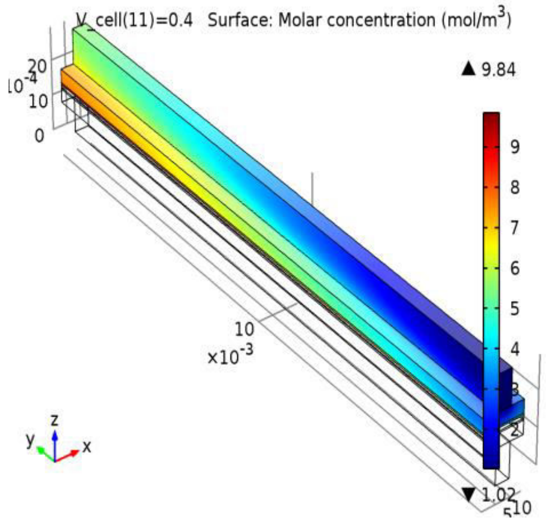

Figure-5. Water concentration at the cathode using cobalt catalyst .Simulations was carried out at operating temperature of 160°C.

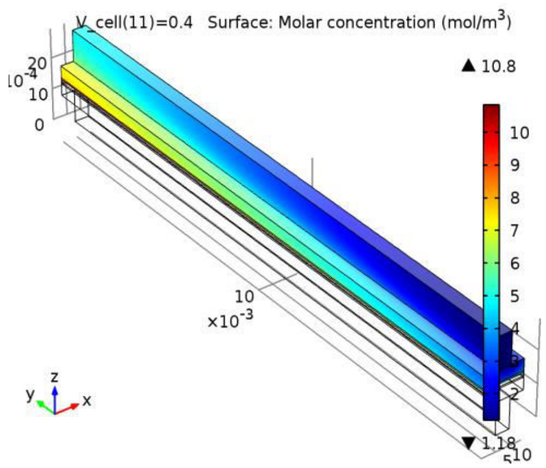

Figure-6. Molar concentration of water at the cathode side of fuel cell at an operating temperature of 120°C for platinum.

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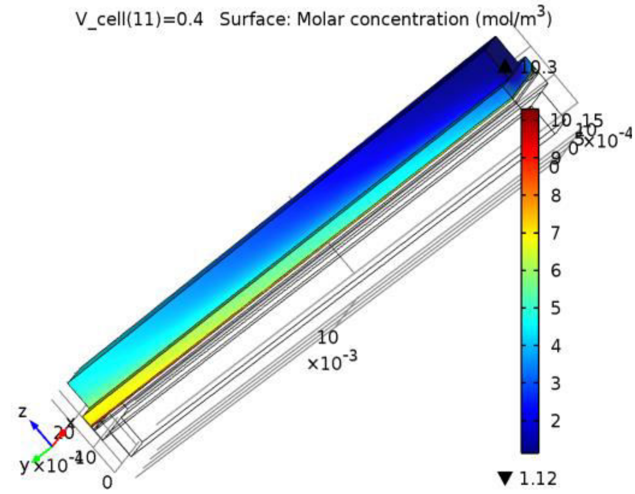

Figure-7. Molar concentration of water at the cathode using cobalt at a temperature of 120°C.

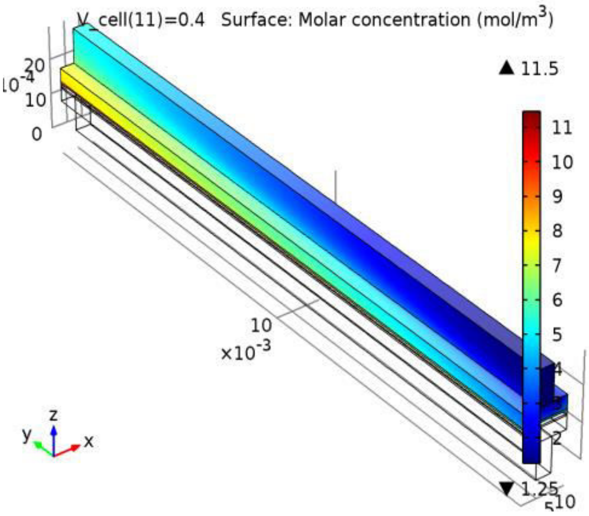

Figure-8. Cathode water concentration in the fuel cell at temperature of 80°C using platinum as a catalyst.

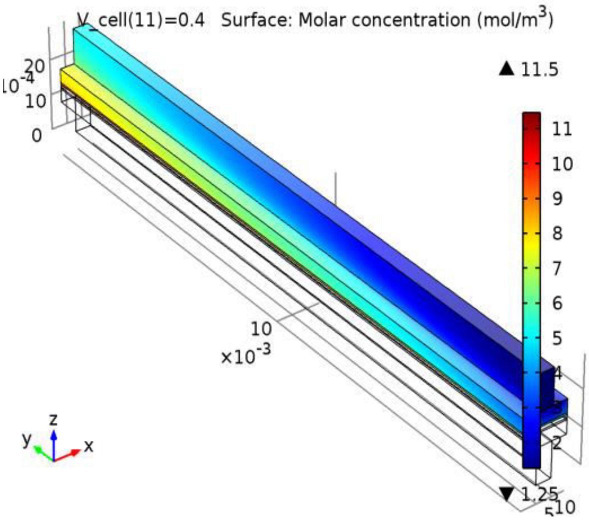

Figure-9. Surface Molar concentration of water at the cathode for a temperature of 80°C using cobalt.

CONCLUSIONS

In this study, a detailed model of a straight channel fuel cell has been presented. The proposed model considers the water accumulation at the cathode side due to the redox reaction inside the fuel cell. Different catalyst has been considered in this study. The results indicated that performance was unaffected even after replacing the catalyst and the membrane by the proposed cost effective material. Further investigations are in progress to investigate electrochemical behavior of the fuel cell when subjected to similar operating conditions.

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