Simulation Of Proton Exchange Membrane Fuel Cell Using Nafion Membranes

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Abstract—In this world of globalization and fantasy, everything starts with the power & finishes with it. So in order to fulfill this hunger of power, fuel cells are the best energy source with negligible fuel cost & without any harmful emission. The fuel cell simulated on this paper is Proton Exchange Membrane fuel cell (PEMFC). The simulation was done by varying different parameters (as membrane thickness, velocity at anode & cathode) and different materials (n-1110, n-115, n-117, n-HP), and it is observed that Nafion-HP is showing better results among all the other n- based membrane materials considering the low average total loss with low concentrated polarization, accordingly the negligible cell voltage drop and the high cathode water concentration.

Keywords— Fuel cell, Simulation, PEM, Nafion, Polarization

I. INTRODUCTION

Fuel cells are one of the cleanest and most efficient technologies for generating electricity. Since there is no combustion, there are none of the pollutants commonly produced by boilers and furnaces. For systems designed to consume hydrogen directly, the only products are electricity, water and heat. Fuel cells are an important technology for a potentially wide variety of applications including on-site electric power for households and commercial buildings; supplemental or auxiliary power to support car, truck and aircraft systems; power for personal, mass and commercial transportation; and the modular addition by utilities of new power generation closely tailored to meet growth in power consumption. These applications will be in a large number of industries worldwide. Fuel Cells (FC) systems are a potentially good clean energy conversion technology and they can be used in a wide variety of power generation applications. There are varieties of fuel cells available in research sector as well as in the market. But the fuel cell we have used for our research is proton exchange membrane fuel cell or polymer electrolyte membrane (PEMFC). The Polymer Electrolyte

Membrane (PEM) fuel cells are currently considered a good candidate for ground vehicle applications and small portable devices as they have high power density, fast startup time as well as long cell and stack life. The essentiality for vehicle with less emission has made PEM fuel cells attractive for vehicular applications since they emit negligible pollutants. The operating parameters are mainly air & hydrogen feed flow and pressure regulation, heat & water management. This work is focused on using different types of membrane materials with varying parameters (i.e. thickness, velocity etc.).

Computational models are now widely used for simulation of the fuel cells behavior and for quantitative estimation of changes in the device performance with system parameters variation. These models can also provide the detailed local data that are frequently unavailable from fuel cell tests.

High temperature proton exchange membrane fuel cells (HT-PEMFCs) with Nafion (n-HP,n-115,n-117,n-1110) - based membrane are considered the next generation of power generating devices due to their superior performance. They operate at higher temperatures from 120 to 153°C and exhibit stable voltage output at steady state conditions. The HT-PEMFC is credited with faster electrochemical kinetics, improved water management, and carbon monoxide tolerance. As a result of the low electro-osmotic drag and the good proton conductivity of the nafion membrane, the fuel cell design and the routine maintenance could also be significantly simplified.

II. MODEL ASSUMPTION

Because the HT-PEMFC is operating above 100°C at around 2 atmospheric pressure, the water exists in vapor form only. Because of the property of the NAFION membranes, the water drag coefficient from anode to cathode is assumed to be zero, which is different from the typical low temperature PEMFC with a PBI membrane. Also, as the membrane is doped with sulphonic acid, the mechanism of proton transfer is through the acid in the membrane. The gas mixture is treated as an ideal gas. The flow is laminar due to the low Reynolds number. The gas diffusion layer (GDL) is made of isotropic and homogeneous porous materials.

III. MODELLING DOMAIN

The 3D computational domain includes a section of the NAFION membranes and both cathode and anode gas flow channels, GDLs, and catalyst layers.

Governing equations - Conservation of mass and momentum. With the preceding assumptions, the HT-PEMFC operation is governed by the following conservation equations.

conservation of mass
$$\nabla \cdot u = \frac{Q}{\rho}$$
 [1]

conservation of momentum

$$\rho u \cdot \nabla u = \nabla \left\{ -pI + \mu [\nabla u + (\nabla u)^T] \right\}$$
[2]

Where u is the gas mixture velocity vector (m/s), ρ is the gas mixture density (kg/m3).

$$\nabla \left\{ -\rho w_i \sum_{j=1}^N D_{ij} \left[\frac{M}{M_j} \left(\nabla w_j + w_j \frac{\nabla M}{M} \right) + (x_j - w_j) \frac{\nabla P}{P} \right] + w_i \rho \vec{u} \right\}$$

= R_i

Q is the source term [kg/ (m3 s)], p is the pressure (N/m2), and μ is the dynamic viscosity of the mixture [kg/ (m s)] and is calculated as:

$$D_{ii} eff = D_{ii}(\varepsilon)^{1.5}$$

In the porous GDL, the pressure drop is proportional to the gas velocity if the flow is laminar, and it is modeled as:

Where K is the permeability of the GDL (m2) and ε is the porosity of the GDL.

$$\mu = \sum x_i \cdot \mu_i$$

IV. CONSERVATION OF ELECTRIC CHARGE

In a PEMFC, the current can be split into two parts: ionic current and electronic current. Protons travel through the ionic conductor (membrane) to form an ionic current, while electrons transfer only through the solid matrix of electrodes, which results in an electronic current. The current continuity equations are obtained by using Ohm's law.

$$(\mu/\kappa)u = \nabla \left\{ -pI + (1/\varepsilon)\mu [\nabla u + (\nabla u)^T] \right\}$$

Where ϕ is the phase potential, σ is the effective electric conductivity (S m-1), S is the current source term (A m-3), and the subscript s denotes the property of the solid phase while m denotes that of the membrane. The source terms in the electron and proton transport equations result from the electrochemical reaction, which occurs only in the catalyst layers of anode and cathode sides, and are given as:

anode side:
$$\eta_a = \varphi_s - \varphi_e$$

cathode side: $\eta_c = \phi_s - \phi_e - U_{oc}$

In the catalyst layers of anode and cathode sides, and are given as:

anode catalyst layer:
$$S_m = j_a$$
 $S_s = -j_a$

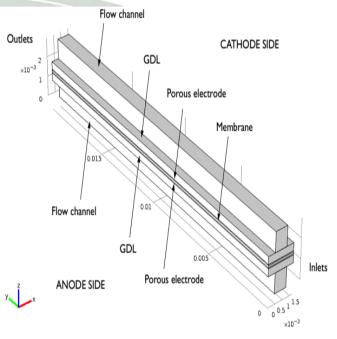
cathode catalyst layer: $S_m = j_c$ $S_s = -j_c$

Where ja and jc are the transfer current density corresponding to the electrochemical reaction at the anode and cathode catalyst layers, respectively.

$$j_{a} = a i_{0,a}^{\text{ref}} \left(\frac{C_{\text{H}_{2}}}{C_{\text{H}_{2},\text{ref}}} \right)^{0.5} \left(\frac{\alpha_{a} + \alpha_{c}}{RT} F \eta_{a} \right)$$
$$j_{c} = a i_{0,c}^{\text{ref}} \left(\frac{C_{\text{O}_{2}}}{C_{\text{O}_{2},\text{ref}}} \right) \exp \left(- \frac{\alpha_{c}}{RT} F \eta_{c} \right)$$

V. DIMENSION OF FUEL CELL

The dimensions of Nafion based membrane PEM Fuel cell are as follows.

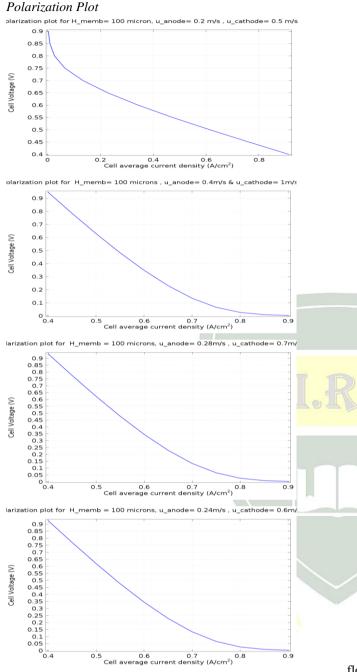


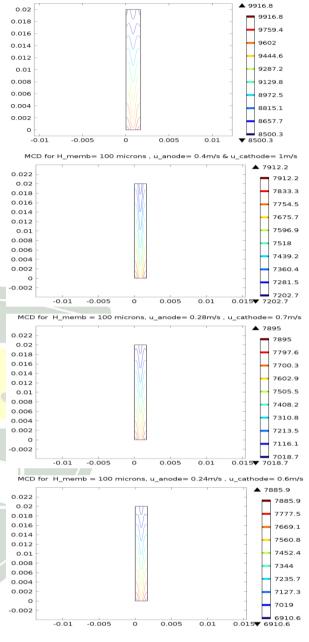
VI. RESULTS AND DISCUSSION

The aforementioned fuel cell model is designed and solved using finite-element-based commercial software COMSOL Multiphysics. A second-order hexahedral element was adopted and a total of 120,513 degrees of freedom was solved using the inbuilt stationary solver.

The following pages will show the simulations and their corresponding results.

Α.



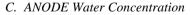


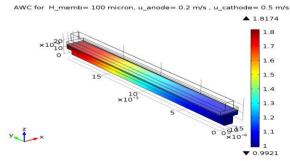
MCD for H_memb= 100 micron, u_anode= 0.2 m/s , u_cathode= 0.5 m/s

a) Inference: It is observed that the activation polarization for Nafion-HP membrane is very less compare to the other membranes (i.e. n-115, n117, n1110) with low gas transport loss i.e. concentration polarization and the total loss of the Nafion – HP membrane is also low compare to other N based membranes.

B. Membrane Current Density

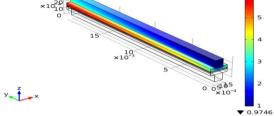
a) Inference: It is observed that, with the increase in flow rate, the cell voltage falls for the same cell average current density across all the three membrane. Although in Nafion – HP based membrane the cell voltage falls negligibly comparing among the other n- based membranes.



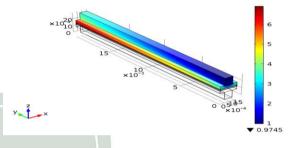


y Z





CWC for H memb = 100 microns, u anode= 0.28m/s, u cathode= 0.7m/s ▲ 6 9175



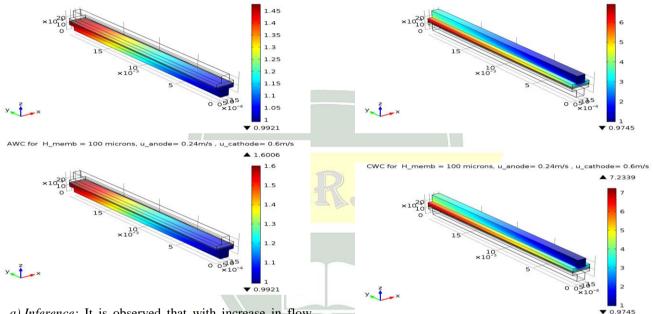
AWC for H_memb = 100 microns, u_anode= 0.28m/s , u_cathode= 0.7m/s ▲ 1.4773

AWC for H_memb= 100 microns , u_anode= 0.4m/s & u_cathode= 1m/s

▲ 1.3022

1.3 1.25 12 1 15 1.1 1.05

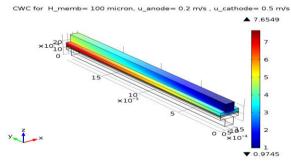
0.9922



a) Inference: It is observed that with increase in flow rates, Anode Water Concentration decreases at inlet only, the concentration though remains constant at the outlet for all the n based membranes. But comparing among the four n-based membranes the Nafion– HP based membrane more concentration fall.

We may conclude for the same flow rate, the anode water concentration decreases with the increase in thickness of the membrane.'

D. CATHODE Water Concentration



a) Inference: With increase in flow rate, the Cathode Water Concentration increases across the outlet but, in inlet, the value of Cathode Water Concentration decreases. But compare to all the other n- based membranes the Nafion – HP based membrane increases negligibly across the outlet then it decreases drastically.

Also, the N- 1110 based membrane has the same comparing factors but never the less, in inlet the concentration is found to be more constant.

We may conclude for the same flow rate, the Cathode Water Concentration decreases with the increase in thickness of the membrane may conclude for the same flow rate, the initial cell voltage falls with a negligible amount, with increase in the thickness of the membrane.

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