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THE EFFECT OF BAFFLE BLOCKS IN A FLOW CHANNEL ON PEMFC CHARACTERISTICS

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ABSTRACT

The aim of this study is to investigate the effects of baffle blocks located in the flow channel on fuel cell characteristics. Parametric study is employed to determine an appropriate number of blocks in flow channel and gap ratio between the blocks on current collector and gas diffusion layer in a single-cell proton exchange membrane fuel cell with baffle-block. No significant effects are observed in polarization curves using higher than four blocks and gap ratio of 0.3..

INTRODUCTION

Fuel cells are among the candidate devices to produce green energy from fossil fuels for the future applications. There are some problems to be overcome during the development of fuel cells. It is needed to increase usage ratio of hydrogen fuel in fuel cells. One of the alternatives is to increase residence time and to use momentum by changing the direction of fuel for effective usage in the fuel cell. It seems this can be done simply placing baffle blocks on the flow path of fuel through the flow channels.

Up to now, limited number of study was conducted on the usage of baffle blocks through the flow channels in fuel cells. One of them belongs to Soong et al. [1] which proposes a novel configuration of partially blocked fuel channel with baffle plates transversely inserted in the channel. The effects of the blockage with various gap ratios and numbers of the baffle plates, the fuel flow Reynolds number and the porosity of the diffusion layer on the reactant gas transport, and the pressure drop across the channel length are explored. The results reveal that reducing the gap size and/or increasing the baffle number to enhance the reactant gas transport results in a penalty of high pressure-loss. With the consideration of both high performance and reasonable pressure drop, the present results disclose that designs with the baffle gap ratio no smaller than 0.1, number of baffle plates N=3-5, and the GDL porosity around 0.7 seem quite appropriate.

The detailed gas transport and cell performance of the PEM fuel cell with baffle-blocked flow field designs are examined by Jang et al [2]. Predictions show that the local transport of the reactant gas, the local current density generation and the cell performance can be enhanced by the presence of the baffles.

Superficial Electrode Area

Theoretical open circuit voltage

NOMENCLATURE

[V]

i	$[A/m^2]$	Local current density				
i_o	$[A/m^2]$	Exchange current density				
i_n	$[m^2K/W]$	Internal current density				
N	[unit]	Number of baffle plates				
V	[V]	Voltage				
X	[m]	Cartesian axis direction				
y	[m]	Cartesian axis direction				
Z	[m]	Cartesian axis direction				
Special characters						
σ	[S/m]	Ionic Conductivity				
Φ	[V]	Phase Potential				
λ	[-]	Gap ratio				
Subscripts						
avg	•	Average				
е		Electrolyte				
0		reference				
Superso	ript					
eff [*]	1	Effective				
Abbrev	iations					
GDL		Gas Diffusion Layer				
MEA		Membrane Electrode Assembly				
PEM		Proton Exchange Membrane				
PEMFO	7	PEM Fuel Cell				

DESCRIPTION OF THE PROBLEM

PEM fuel cell is composed of eleven elements as shown in the detailed views of flow channels and pre-assembly; five of them on the anode side and the others symmetrically placed on the cathode side, say, anode and cathode catalyst layers (5,5'), gas diffusion layers (4,4'), gas channels (3,3'), baffle blocks (2,2'), bipolar current collectors (1,1') and membrane (6) on the symmetry plane. Solution domain is the whole cell geometry including anode and cathode sides. Baffle blocks are attached to the current collector faces at the midpoint of gas channels.

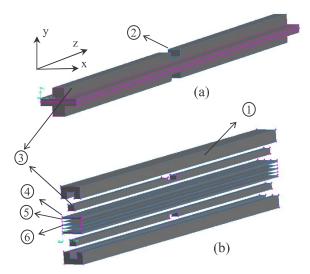


Figure 1 PEM Fuel Cell view from Fluent-Gambit module:
a) Isometric view of flow channels with MEA
b) Pre-assembly of complete cell.

Membrane Electrode Assembly (MEA) including membrane, catalyst layers and gas diffusion layers has an active surface area of 0.21 cm². Total cell volume - width, height and length-is 3 x 4.7 x 70 mm³. Electrochemical parameters needed in PEMFC module of Fluent are presented in Table 1. Material for catalyst layers is selected as platinum due to low operational temperature in PEM fuel cell's and to increase the electrochemical reaction rate on the anode and cathode sides. Material for bipolar plate is selected as graphite due to high electrical conductivity. TGP-H-060 is used as gas diffusion layer. Catalyst layers have combined properties of graphite and platinum materials. Nafion is used as membrane material.

MATHEMATICAL MODEL

A 3-D single fuel cell model was used to simulate the transport phenomena inside the PEMFC. Governing equations of continuity, momentum, energy, and species concentrations of different components of a fuel cell, as well as the equations for phase potential in the membrane and the catalyst layer are coupled with chemical reaction kinetics by introducing source terms. Details of the model can be found in Alpat's study [3]. In this work, the computational domain consists of three-dimensional complete fuel cell. The assumptions used in

developing the model are the same in the PEM fuel cell module of Fluent.

Table 1. Electrochemical parameters [4]

Electrochemical Parameters	Values
Anode ref. current density	$1.0 \times 10^9 \text{ A m}^{-3}$
Anode ref. molar concentr.	0,546 kmol m ⁻³
Anode concentr. exponent	0,25
Anode exchange coeff.	1,5
Cathode ref. current density	20000 A m ⁻³
Cathode ref. molar concentr.	0,00339 kmol m ⁻³
Cathode concentr. exponent	0,5
Cathode exchange coeff.	2
Open circuit voltage	1,18 V
Hidrogen ref. diffusivity	$7,33 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$
Oxygen ref. diffusivity	$2,13 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$
Water ref. diffusivity	$7,33 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$
Species ref. diffusivity	$4,90 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$

The fuel cell operation is governed by the mass, momentum, species and charge conservation equations. The conservation equations of mass, momentum, species and charge that are suited for Fluent using a single domain formulation. The details can be found in the thesis of Öztoprak [4].

The local current density is calculated as:

$$i(x,z) = \sigma_e^{eff} \frac{\partial \Phi_e}{\partial x} \tag{1}$$

and the average current density [9] is

$$i_{avg} = \frac{1}{A} \iint_{A} i(x, z) dx dz \tag{2}$$

Conservation of mass, momentum and energy are solved in gas channels and diffusion layers. Conservation of momentum for porous media is reduced to Darcy Law.

In PEM fuel cell model, the solution is obtained assuming chemical reactions to be heterogeneous and to occur on the side of catalyst facing to membrane. Potential difference between the catalyst layers and the membrane is driving force for the reaction to occur and is called as activation loss or surface overpotential. The potential difference between the anode and cathode current collectors is called as an external-circuit voltage. Current transfer on the catalyst layers is calculated using Butler-Volmer equality. Two electric potential fields are solved in the model. The first is solved in the membrane and catalyst layers and the other in the catalyst layers, the diffusion layers, and the current collectors. Surface reactions on the porous catalyst region are solved and the reaction diffusion balance is applied to compute the rates. The current density value is computed based on the prescribed cell voltage value.

Boundary Conditions

In this study, "mass flow inlet" and "pressure outlet" boundary conditions are attained at the inlet and outlet ports of the anode and cathode gas channels respectively. The "wall" boundary condition is attained at the surfaces of current collector that faces with the gas channels and outside air. The "porous jump" boundary condition is attained at the interface between membrane and catalyst layers, and between gas diffusion layers and gas channels. The details of boundary conditions that is attained to the surfaces of each layer of the PEM fuel cell can be found in Öztoprak's thesis[4]

NUMERICAL METHOD

Hexagonal grids are used in the construction of mesh structure. Control volume approach is used in the discretization of conservation equations in integral form. First order upwind method is used in the discretization of convective terms. Implicit pressure based (segregated) scheme (SIMPLE algorithm) and Gauss-Seidel iterative technique (segregated solver) is used in the solution of set of algebraic equations. The under-relaxation parameters for momentum and pressure are selected as 0.3 to slow down the speed of convergence. It is assumed that converged solution is obtained when the residual value for energy and all the other solved properties reach to 10^{-6} and 10^{-4} , respectively.

Grid independency tests

Grid independency tests were performed to obtain optimum number of grid points. For this purpose, five different distributions of element numbers were determined varying interval size of grid structure as shown in Table 2.

Table 2 Variation of mean current density and solution time

with mesh number						
Interval Size	Total no. of Mesh	Current Density (A cm ⁻²)	Dev. in Current Density (%)	Solution Time (min)		
0,6	7722	0,103897	-	4		
0,5	10920	0,104735	0,80	6		
0,4	18900	0,104156	0,56	10		
0,2	131250	0,104131	0,03	84		
0,15	323631	0,109293	4,72	242		

Tests were performed at atmospheric pressure for cell potential of 0.88 V. Other operational parameters are selected as follows; Hydrogen and water vapour mixture is fed to the anode gas channels at a mass flux of 3.10×10^{-6} kg/s and at a mass fraction of 0.11 for H_2 and 0.89 for H_2O . Humidified air is fed to the cathode gas channels at a mass flux of 1.58×10^{-6} kg/s. Oxygen and water vapour mass fractions are taken as 0.15 and 0.36 in the air, respectively.

It can be thought that the correct result was caught when the minimum change was observed in the current density for successive grid results and this point corresponds to 131250 grid numbers in the problem. But, one must also take into account the solution time. Combination of the effects of current density change and the solution time help us to determine the proper grid number such as 18900 in this problem.

RESULTS

Results are presented as polarization curves. The following sections explain the methodology in construction of the

polarization curves and determination of block height and number.

Construction of Polarization Curves

Total cell over-potential is defined as the difference between the theoretical open cell voltage and cell voltage. Therefore, each of the cell over-potential corresponds to a cell voltage. Current density values are computed from the numerical model corresponding to the over-potential values (cell voltage). Total cell over-potential is increased by step function like a hyperbolic relaxation function [5]. Seven over-potential steps are determined as 0.23, 0.28, 0.33, 0.38, 0.58, 0.78, and 0.88. The polarisation curve is constructed using the computed current density values and cell voltage values for these seven steps [4]. The results reached from a converged solution are taken as initial values for the solved quantities at the next solution step.

Open circuit voltage is calculated as 0.92 V using the Tafel equation below [6],

$$V = E - A \ln \left(\frac{i + i_n}{i_o} \right) \tag{3}$$

Where i_o and i_n represent exchange current density and internal current density, respectively. E is called theoretical open circuit voltage when no current passes through the circuit. The value of theoretical open circuit voltage is calculated as 1.18 for the fuel cell taking the fuel cell parameters [4] such as reference current density ($i_o = 0.04 \text{ mAcm}^{-2}$), crossover current ($i_n = 3 \text{ mA} \text{ cm}^{-2}$) and coefficient in Tafel equation (A=0.06 V) for the fuel cell studied.

Determination of the block height and number

In this study, to determine the block height that maximize the current density produced, six different gap ratios, λ which is the ratio of gap between the block tip and channel wall to the channel height are selected as $\lambda = 0.1, 0.2, 0.3, 0.4, 0.5$ and 1.0. Polarization curves are constructed for the gap ratios with and without blockage ($\lambda = 1.0$). In these trials, the operational parameters are taken the same as in the grid independency tests. The results are presented in Figure 2.

The highest and the lowest values of the current density are obtained for gap ratio of 0.1 and 1, respectively. The current density values for gap ratios of 0.3, 0.2 and 0.1 are much closer to each other, and there is a discrepancy between the current density values for gap ratios of 0.3 and 0.4. It is thought that it may be reasonable to study with the gap ratio of 0.3 only. Therefore, it is continued to study with gap ratio of 0.3 to determine an appropriate number of baffle blocks that maximizes the current density. The results are presented in Figure 3 to show the effect of the number of block on the current density and cell voltage. It is clearly shown on the Figure that there is no need to use block number higher than 4 because they produce the same current density value.

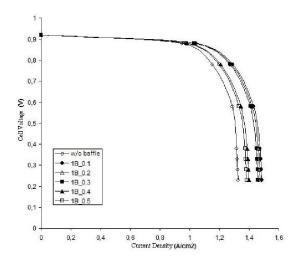


Figure 2 Polarization curves for different gap ratios

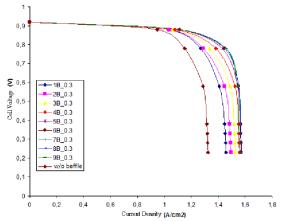


Figure 3 Polarization curves for different block numbers

CONCLUSION

Numerical results indicate that placing baffle blocks in the flow channel of PEM fuel cell increases cell current density. Nevertheless, there should be an upper limit of cell current density due to physical restrictions and it seems around the value of 1.58 A/cm² as shown in Figure 3. The parameters satisfying this maximum attainable current density value is obtained at the condition of placing 4 baffle blocks and selecting gap ratio of 0.3

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