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Numerical Predictions of Oxygen Transport Enhancement in a PEM Fuel Cell with Flow Field Designs

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Abstract: Present study investigates the cathode gas channel of proton exchange membrane fuel cell that is partially blocked by one or more baffle plates. In order to investigate the effects of the selected shape, size and the number of baffles on oxygen transport in the gas diffusion layer a numerical modeling is carried out in 27 cases. With consideration of both maximum oxygen concentration in the gas diffusion layerand reasonable pressure drop, the results indicate that in all cases, an increase in baffle height is more effective than an increase in number of baffle plates. Also, installing three large rectangular baffles seem quite appropriate, but when there is restriction in securing pressure in fuel cell, installing the semicircle baffle is better than the rectangular one.

Key words: PEMfuel cell; Baffles・Oxygen transport・Pressure drop・Channel blocking

INTRODUCTION

The bipolar collector/separator plates in a PEM fuel cell stack typically include separate flow channels to supply hydrogen and oxygen reactant gases to anode and cathode electrodes. The flow field geometry is one of the most important enhancing factors forgases transportedfrom GDLs into catalyst layers. Most PEM fuel cells made to date use straight gas flow channel configurations, whereas serpentine flow channels and inter-digitized flow field are commonly used in many fuel cell flow field designs. Recently, several studies have attempted to improve PEM fuel cell performance through flow field design such as straight [1-5], serpentine [6-9] and many other novel combinations [10] of these conventional types. In addition to flow pattern, an effective design of gas flow field, through optimization of the channel dimensions and configuration, may result in an improved bipolar plate. Partially blocked channels with baffle plates being transversely inserted in the channels can increase the reactant gases flow rate to the catalyst layer and the removal of water vapor produced; therefore, PEM fuel cell performance is improved. Liu *et al*. [11] employed two dimensional model of a PEM fuel cell to investigate the effect of blocking of gas flow channel with rectangular baffle plate(s) on current density. They showed that the local transport of the reactant gas, local current density generation and the cell performance can be enhanced by the presence of the baffle. Perng *et al*. [12] have simulated cathode gas channel with rectangular cylinder in the channel and also have investigated the effects of the blockage at various gap sizes and the width of the cylinder on the cell performance enhancement. Soong *et al*. [13] have investigated the effect of cathode channel blocking in PEM fuel cell with one or several rectangular baffles. From the literature survey stated above, it is clear that very few studies have investigated the effect of baffle shape, size and number of baffles on gas transport into GDL and effective area of catalyst layer. Moreover, little attention has been given to the optimization of channel blocking in order to create the most oxygen diffusion in GDL and less pressure drop in the cell.

In order to enhance cell performance, this study i) proposes a new configuration of partially blocked oxygen channel ii) investigates the effect of blocking with various shapes of baffle plate consisting of rectangular, triangle and semicircle plates on oxygen transport; iii) explores the

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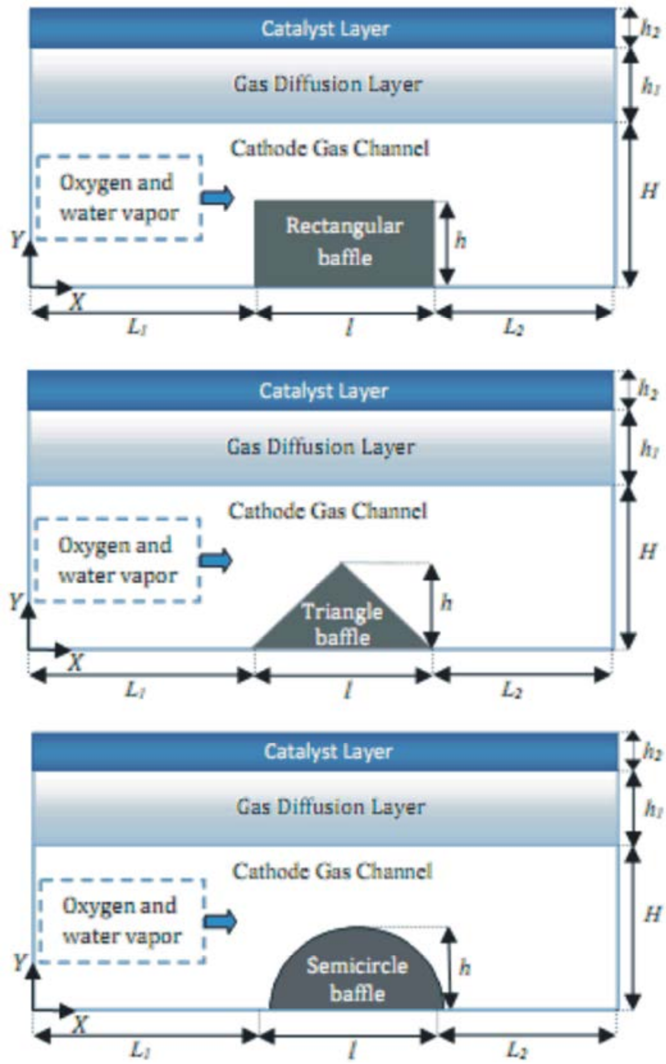

Fig. 1: Two-dimensional geometry and computational modeling for PEM fuel cell cathode. Three cases for blocking with plate(s), equal length in amidst of channel

influence of the blockage with various sizes and numbers of plates in the channel on the oxygen diffusion in GDL; iv) evaluates the pressure drop in the presence of various blockage effects; and v) proposes the best configuration of partially blocked channel to have maximum oxygen transfer in the GDL and minimum pressure drop in the cell. A two-dimensional and single-domain is modeled to investigate the velocity field, the oxygen flow rate reaching at the GDL layer, the concentration of water vapor produced and the pressure drop at various conditions of the baffle plates in the oxygen channel of a PEM fuel cell.

Mathematical Modeling: The model domain consists of the following subregions: the gas channel, gas diffusion layer and catalyst layer for the cathode side, with rectangular, triangle or semicircle baffle plate(s) along the transverse section of the flow channel as shown in Fig. 1. The parameters h, H, H-h, h_1 and h_2 depict the baffle height, flow channel height, gap size, GDL thickness and catalyst thickness, respectively. The channel length is $L = L_1 + l + L_2$ with l, L_1 and L_2 standing for the thickness of the baffle plate, the upstream and downstream channel lengths, respectively. Air flow through channel is distributed into cathode. Oxygen reduction reactions occur only within the active catalyst layer.

Assumptions: The following assumptions are made in implementing the single-phase model: (i) two-dimensional, (ii) steadystate flow, (iii) ideal gas mixtures, (iv) laminar

Table 1: Governing equations for two-dimensional model

Conservation equation		Source terms	Number of equation
Mass	$\nabla.(\varepsilon\rho\vec{u})=0$	-	(1)
Momentum	$\frac{1}{\varepsilon^2}\nabla.(\rho\vec{u}\vec{u})=-\nabla p+\nabla.(\mu\nabla\vec{u})+S_u$	$S_u=-\frac{\mu}{K}\vec{u}$	(2)
Species	$\nabla.(\vec{u}C^i)=\nabla.(D^{i,eff}\nabla C^i)+S_k=0$	$S_{k,O2}=-\frac{I}{4F}M_{O2}$ $S_{k,H_2O}=\frac{I}{2F}M_{H_2O}$	(3)

and incompressible flow with low Reynolds numbers and pressure gradients, (v) no contact resistance at the interfaces between GDL and catalyst layers, (vi) constant viscosity of gas mixture is calculated for the inlet condition and (vii) the operating temperature of fuel cell is 80°C.

Governing Equations: In contrast to the usual approach which employs a separate differential for different sub-regions, here a unified single-domain approach with a single set of governing equations is applied to all sub-regions. In the developed single-domain method, one set of conservation equations is considered for different regions of PEM fuel cell cathode electrode [14]. Thus, under the above mentioned assumption, the model has a set of coupled non-linear partial differential equationsincluding conservations of mass, momentum and species. The relevant equations are presented in Table 1. In these equations, $\vec{u}$, ρ, p, μ and ε are mixture velocity, density, pressure, gas mixtureviscosity andvolume fraction of GDL respectively. The C^i is the total concentration of species I and $D^{i,eff}$ is the effective diffusivity of species i in gas mixture. Diffusivity in channel is a function of pressure and temperature [15].

The source term of momentum equation, Eq. 2, is employed to consider Darcy's law under the limiting condition [16]. The proportionality factor K in Darcy's model is the permeability of the porous medium. The source terms in the species conservation equation, S_k, is equal to zero everywhere except in the catalyst layer, where the species are consumed or generated in the electrochemical reactions. Also, I is the current density and F is Faraday constant. The distribution of current density is characterized by a descending trend along the channel length due to oxygen consumption with axial location X. In the present study, the current density distribution was obtained from measured experimental data presented by Perng *et al*. [12].

Table 2: Physical and dimensional parameters and transport and material properties

Description	Unit	Value
Dimensional parameters		
Baffle height, h	mm	0.15, 0.25, 0.35
Flow channel height, H	mm	0.5
Gap size, H-h	mm	0.35, 0.25, 0.15
Gas diffusion layer thickness, h_1	mm	0.2
Catalyst thickness, h_2	μm	10
Flow channel length, L	mm	10
Baffle plate thickness, l	mm	2
Upstream channel length, L_1	mm	4
Downstream channel length, L_2	mm	4
Operating conditions		
Cell temperature, T	K	353.15
Cathode pressure, P	atm	1
Cathode stoichiometry		1.1
Cathode dry gas mole fraction		79
Transport parameters		
Faraday's constant, F	C/mol	96487
Cathode gas viscosity, μ	Pa.s	1.88×10^{-5}
O_2 diffusivity in the cathode gas channel, D	m^2/s	1.81×10^{-5}
H_2O diffusivity in the cathode gas channel, D	m^2/s	2.236×10^{-5}
Material properties		
GDL and catalyst layer porosity, ε		0.6
GDL and catalyst layer permeability, K	m^2	10^{-12}

Boundary Conditions: Equations of conservations of mass, momentum and species, form a complete set of governing equations for four unknowns: u, v, p and C^i. Solving these equations needs to specify the suitable boundary conditions. No-flux condition is applied to the equations for flow and transport at all boundaries except inlet and outlet channel. The inlet velocity in the gas channel is expressed by the respective stoichiometric flow ratio. In this model, inlet velocity is considered 1 meter per second. Fully developed flow with a given back pressure is assumed to take place at the outlet.

Numerical Procedures: The geometry is given in Fig. 1 with the specifications listed in Table 2. The governing equations were discretized using a finite-volume method and solved using a computational fluid dynamic code.

The pressure and velocity fields are treated with the SIMPLE pressure correction algorithm, where a single-domain model is used. Stringent numerical tests were carried out to ensure that the solution was independent of grid size. 200 grids along the channel and 50, 40 and 10 grids along the thickness of each channel width, GDL and catalyst layer were used respectively. The coupled set of equations was solved iteratively and the solution was checked to be convergent when the relative error in each field between the two consecutive iterations was less than 10^{-6}.

RESULTS AND DISCUSSION

For validation purpose, the axial velocity distribution from this model at midway of the gap region (X/L = 0.5) is compared with analytical results, as shown in Fig. 2. For the small values of the porosity, the Darcy law gives a uniform flow solution in porous layer. So, the obtained results from this model show a very good agreement with the analytical results and deviation is less than 5%. Also, the maximum pressure drop across the channel length obtained from the case without blocking plates is compared with analytical data for laminar flow in square channel that is as follows:

$$\Delta P = f\frac{l}{d}\frac{V^2}{2} \tag{4}$$

where f, L, d and vare friction coefficient, channel length, hydraulic diameter and average velocity in channel where the Reynolds number is about 29. The deviation between maximum pressure drops obtained from Eq. (4) (about 14.1Pa) and the present numerical study (about 12Pa) is less than 14.5%.The deviation could be as a result of 2D modeling, where inlet velocity instead of average velocity in Eq. (4) and simplified assumption on analytic correlation are used.

In a PEM fuel cell with the cathode channel being partially blocked by installing baffle plate, the presence of the baffle plates has a significant impact on the flow field in the channel and the gas reactant transport through the GDL to the catalyst layer. Flow velocity along the channel in the cathode GDL/catalyst layer interface and oxygen concentration in this interface is shown in Figs. 3 and 4. An abrupt change of velocity occurs at the gap region and the gas flow is forced into the GDL by the installation of a rectangular plate in the flow channel. This causesa larger amount of oxygen to move into the GDL around the region abovethe platetherefore, the reaction at the catalyst layer can be enhanced. The oxygen concentration is decreased along the channel due to the consumption at cathode catalyst layer, but at downstream channel length with baffle plate, the oxygen concentration is more than oxygen concentration in the channel without plate. However, the baffle plate causes a larger pressure dropand needs a higher pumping power for delivery of the oxygen. The maximum pressure drop is about 4 times the case without a plate.

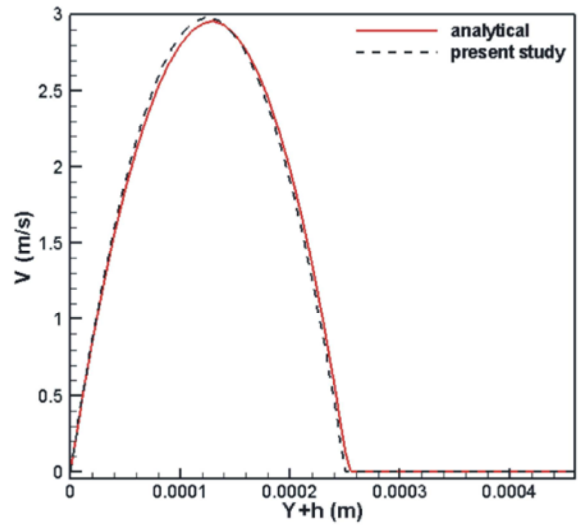

Fig. 2: Comparison of numerical and analytical results of axial velocity distributions in the gap region GDL layer

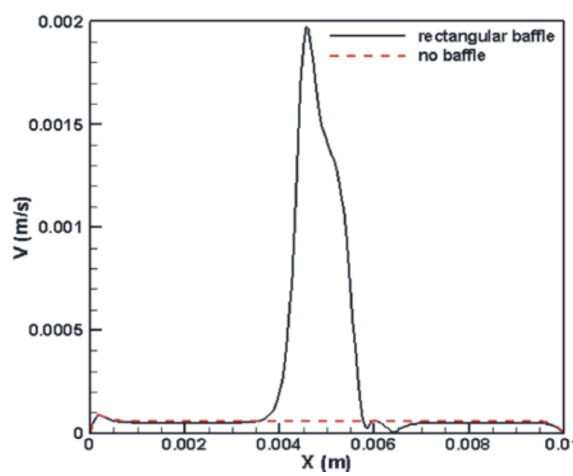

Fig. 3: Comparison flow velocity in the cathode GDL/catalyst layer interface along the channel between cases with and without rectangular baffle in the channel

An appropriate design of the flow channel has been reached by installed baffle plate(s) with various shapes, sizes, numbers and locations of plates in the channel.

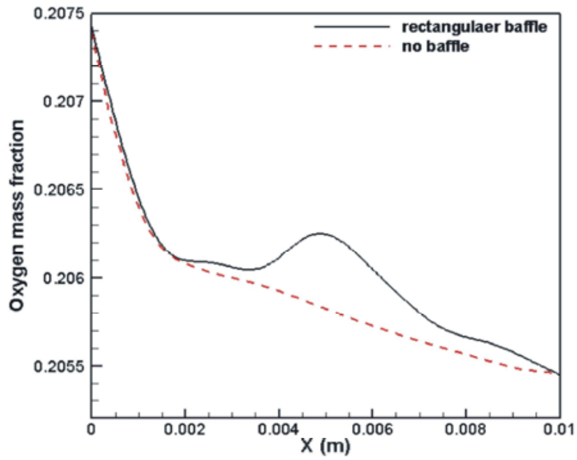

Fig. 4: Comparison, oxygen concentration in the cathode GDL/catalyst layer interface along the channel between cases with and without rectangular baffle in the channel

It can be expected that the change in the parameters mentioned may have a considerable influence on the mass transport. With the consideration of both maximum of oxygen concentration in the gas diffusion layer (or maximum velocity) and minimum pressure drop, we define a dimensionless number called CHB, an abbreviated channel blocking, to arrive at a better quantified evaluation of the effects of installation of baffle plate(s).

$$CHB = \frac{\Delta P}{\rho \overline{V}^2} \quad (5)$$

ΔP is pressure drop along channel, ρ is gas (oxygen) density and $\overline{V}$ is average velocity of reactant gases in the cathode GDL/catalyst layer interface, which is defined as follows:

$$\overline{V} = \frac{1}{L}\int_0^L V dx \quad (6)$$

where L is channel length and V is velocity distribution along the channel in the cathode GDL/catalyst layer interface.

It should be noted that channel should be designed to have smaller CHB value. In this work, we investigatedthe effect of shape of baffle plate thatconsisted of rectangular, triangle and semicircle baffle on the oxygen transfer in the GDL and pressure drop in the cathode side. For each shape, the effect of size and number of plates in the channel was investigated. Therefore, modeling was accomplished for 27 different cases. Table 3 shows the results of numerical solution of fuel cell cathode for 27 blocking cases. As can be seen in this table, with the increase in plate(s) height and also the number of blocking plates, when the shape is specific, average velocity in the cathode GDL layer/catalyst layer interface is increased; however in these cases, the pressure loss is increased, requiring a higher pumping power for the delivery of the oxygen too. As the velocity is increased, more oxygen enters the GDL layer and the oxygen concentration is increased obviously in this layer and catalyst layer. The reaction at the catalyst surface is enhanced with more oxygen supplied. By comparison of cases 1, 10 and 19, which investigate the effects of shape, it is observed that the least CHB is for rectangle, semicircle and triangle baffle, respectively. However, in case 9, the three large rectangular plates, the pressure drop is the most. Also, in all cases, the effect of the increase in plate height is more remarkable than the increase in the number of plates on the CHB. The rank of each of 27 cases of optimum performance (smaller CHB value) is shown in the seventh column. The results indicate that the blocked channel with three large rectangular baffles, case 9, gives the least CHB and therefore, the mostoptimal blocking plate. So, this willresult in an optimumcondition.

Table 3: The results of fuel cell cathode velocity and pressure drop for 27 blocking cases

Shape, height and number of baffles	No. blocking case	baffle height (mm)	Pressure drop (Pa)	$\overline{V}\times 10^5$ (m/s)	CHB× 10^9	Rank
	1	0.15	13.9	7.0254	2.816	22
	2	0.15	15.3	7.8002	2.515	20
	3	0.15	17.3	8.9208	2.174	16
	4	0.25	18.8	9.8533	1.936	14
	5	0.25	26.5	14.3010	1.296	9
	6	0.25	43.3	18.4668	0.966	7
	7	0.35	42	23.6994	0.748	5
	8	0.35	86.5	50.1282	0.344	2
	9	0.35	125	72.4184	0.238	1
	10	0.15	13.6	6.7830	2.956	24
	11	0.15	14.1	6.3072	3.544	27
	12	0.15	14.9	6.8340	3.190	26
	13	0.25	15	6.8781	3.171	25
	14	0.25	15.5	7.9180	2.472	19
	15	0.25	18.1	9.4356	2.033	15
	16	0.35	19.8	10.2975	1.867	13
	17	0.35	32.1	16.8530	1.130	8
	18	0.35	37.5	20.7513	0.871	6
	19	0.15	13.6	6.7891	2.951	23
	20	0.15	14.7	7.4361	2.658	21
	21	0.15	16.1	8.2196	2.383	18
	22	0.25	16.5	8.4676	2.301	17
	23	0.25	21	11.0498	1.720	12
	24	0.25	25.9	13.8864	1.342	10
	25	0.35	22.8	12.3	1.507	11
	26	0.35	46.4	25.2988	0.725	4
	27	0.35	63.5	35.3157	0.509	3

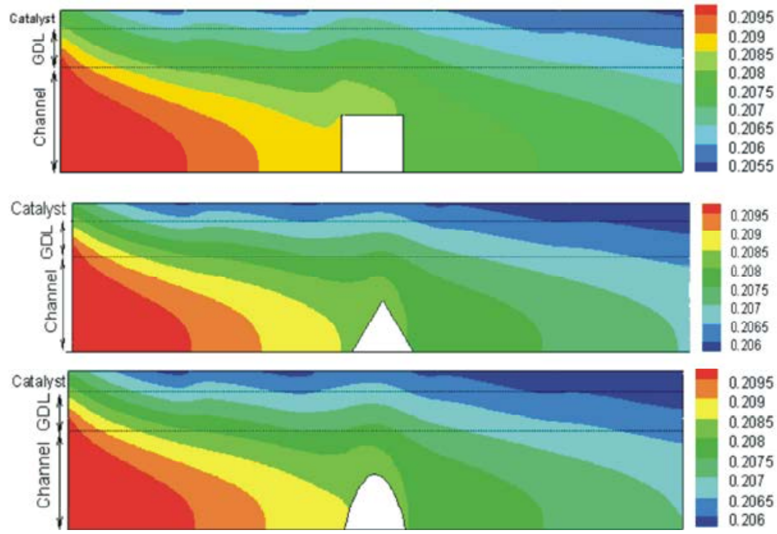

Fig. 5: Oxygen concentration contour for three blocking cases with rectangular, triangle and semicircle baffles

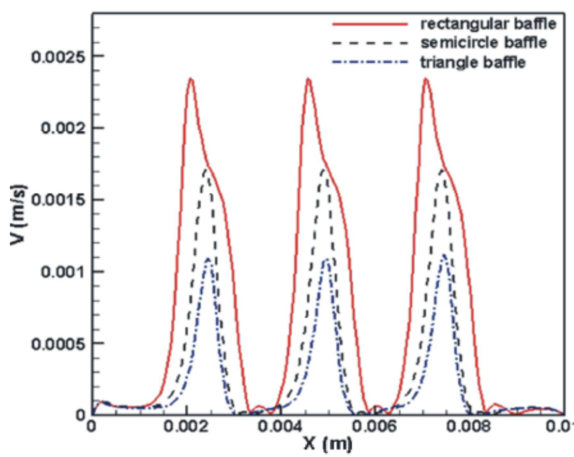

Fig. 6: Velocity distribution in the GDL/catalyst layer interface, three rectangular baffles, three semicircle baffles, three triangle baffles

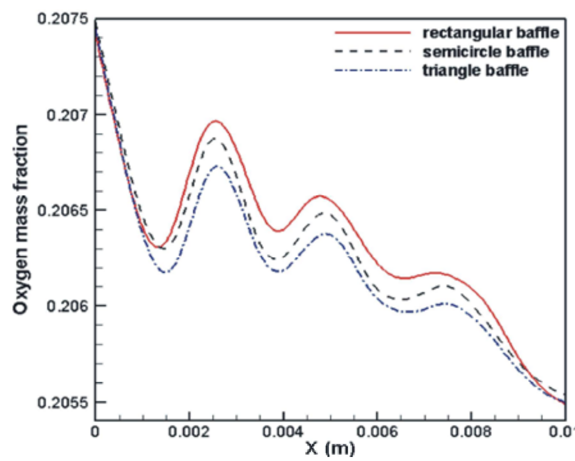

Fig. 7: Oxygen concentration distribution in the GDL/catalyst layer interface, three rectangular baffles, three semicircle baffles, three triangle baffles

Even with reducing the number of large rectangular plates, CHB obtained from two large rectangular baffles plate, case 8, is smaller than the other cases. Installing two large rectangular baffles is allocated to rank 2. With installing three large semicircle baffles, case 27, CHB is slightly higher than case 9, but the pressure drop is much lower. The apparent pressure drops increase the pumping power requirement for operating a fuel cell system. So, when there is restriction in the pumping power, installing the semicircle baffle is better than the rectangular baffle. By installing the triangle baffle, the CHB number will increase significantly. So installing triangle baffle does not seem to be appropriate.

Fig. 5 illustratesoxygen concentration in cathode for threebaffle shapes consisting of rectangle, triangle and semicircle plate. The maximum oxygen concentration in GDL layer occurs beneath the rectangular plate. The effects of baffleshape type on velocity distribution, oxygen concentration in GDL/catalyst layer interface and pressure drop along the channel are shown in Figs. 6, 7 and 8, respectively. In these figures, three rectangular baffles, three semicircle baffles and three triangle baffles areinstalled in flow channel. The maximum velocity in the gap region between GDL and baffle occurs by installing rectangular baffle(s) and minimum velocity is with triangle baffle. Oxygen concentration in catalyst layer along this gap is increased with increasing the velocity. However, corresponding to Fig. 8, pressure drops is the result of increasing velocity beneath plates and GDL.

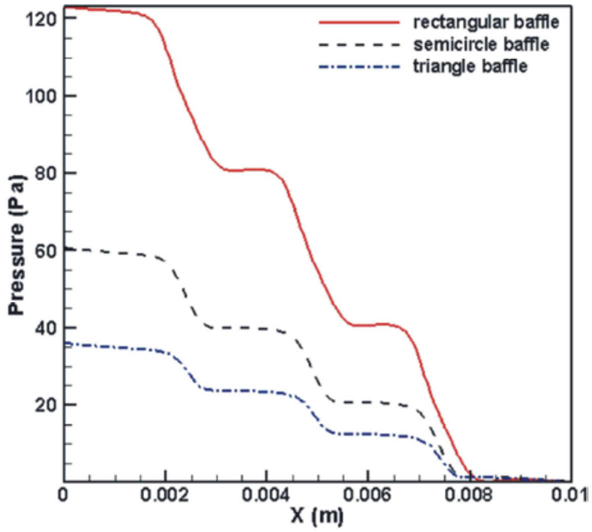

Fig. 8: Pressure variation along the channel, three rectangular baffles, three semicircle baffles, three triangle baffles

CONCLUSIONS

A two dimensional model has been developed for a PEMFCcathode with partially blocked channel to investigate the effect of plate shape, size and the number of baffles on transport phenomena in gas diffusion layer. The following conclusions are drawn:

- By installing the baffle plate, flow velocity in the gap between the baffle and the GDL isincreased; causing more oxygen to bediffused into GDL and increasingreaction rate in catalyst layer, however, pressure drop along the channel is increased too. Therefore, it should be chosen as optimum case. ii) To compare different blocking cases, we introduced a dimensionless number as theratio between pressure and squaredvelocity and called CHB.iii) According to CHB definition, the best blocking case between 27 investigated cases is installing three rectangular baffles with the height of 0.35 mm. iv) By installing three semicircle baffles with the height 0.35 mm, CHB number was found to be slightlyhigher thanits valueinthe bestcondition,but the pressure drop was much lower. So when there is restriction in securing pressure in fuel cell, installing the semicircle baffle is better than the rectangular one. v) By the increase in the number of baffles and baffle height, CHB is decreased. CHB is more sensitivethan theheight.

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Persian Abstract

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چکیده

در این تحقیق کاتد کانال گازی با غشای تبادل پروتون پیل سوختی که توسط بافل بلوکه شده است مورد بررسی قرار گرفت. اثر شکل، اندازه و تعداد بافلها در انتقال اکسیژن در لایه نفوذ گاز، مدل عددی برای ۲۷ مورد بررسی گردید. با لحاظ نمودن حداکثر غلظت اکسیژن در لایه نفوذ گاز و افت فشار معقول نتایج نشان داده است که در کلیه موارد تاثیر افزایش ارتفاع بافل بیشتر از اثر تعداد بافلها بوده است. گرچه نصب سه بافل مستطیلی بنظر مناسب می‌رسد ولی هنگامیکه محدویت در تامین فشار در پیل سوختی وجود دارد نصب بافل نیم دایره ای بهتر از بافل مستطیلی است.