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Numerical Optimization Design of PEM Fuel Cell Performance Applying the Taguchi Method

Shan-Jen Cheng, Jr-Ming Miao, Sheng-Ju Wu

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***Abstract*—**The purpose of this paper is applied Taguchi method on the optimization for PEMFC performance, and a representative Computational Fluid Dynamics (CFD) model is selectively performed for statistical analysis. The studied factors in this paper are pressure of fuel cell, operating temperature, the relative humidity of anode and cathode, porosity of gas diffusion electrode (GDE) and conductivity of GDE. The optimal combination for maximum power density is gained by using a three-level statistical method. The results confirmed that the robustness of the optimum design parameters influencing the performance of fuel cell are founded by pressure of fuel cell, 3atm; operating temperature, 353K; the relative humidity of anode, 50%; conductivity of GDE, 1000 S/m, but the relative humidity of cathode and porosity of GDE are pooled as error due to a small sum of squares. The present simulation results give designers the ideas ratify the effectiveness of the proposed robust design methodology for the performance of fuel cell.

***Keywords*—**PEMFC, numerical simulation, optimization, Taguchi method.

I. Introduction

FUEL cells are regarded as a promising and environmentally friendly power generation for power of electric vehicles, modular design of cellular phone and distributed residential power generation. At the possible alternative power sources, proton exchange membrane fuel cells have high energy density at low operating temperature, quick start-up capability, a pollution or noise free character. They are directly transformed the chemical fuel cell energy into electricity in electrochemical reactions, but still are more expensive than traditional internal combustion engines. Due to the performance of PEMFC is determined by many parameters, such as pressure of fuel cell, operating temperature, the relative humidity, porosity and conductivity of GDE. However, in order to improve performance of fuel cell and the cost more efforts are essential to investigate the physical characteristic effect on the operating conditions [1].

A number of open literatures have been discussed the parameters effect in reference to the present study. Amirinejad et al. [2] investigated the parameter effects such as temperatures, pressures and gas humidity on the performance of PEMFC using experiments. Berning et al. [3] used CFD software to consider the effect of operating pressure and temperatures as well as GDE porosity and thickness on the PEMFC performance. Santarelli et al. [4] studied experimentally different operation variables as like： both cell and flow temperature, reactant pressure on the characterization of cell. Wang et al. [5] studied experimentally individual different operating parameters effects on the performance of PEMFC. Guvelioglu et al. [6] studied the cell performance in different flow rate and humidity with two-dimensional CFD.

From the survey literature of studies were focused on the parameter study of the effects of physical variables at one time. To evaluate the influence of a single parameter is difficult when other properties are kept constant. The experimental data can only observe the average current density, but cannot realize the physical phenomena of inner part through experiment. However, the method of optimization by experimental is time consuming and expensive compared to the numerical optimization, which can yield the global optimization since many parameters can be simultaneously varied [7-8]. So numerical modeling can help realizing of the physical properties within the fuel cell. It is a very useful tool for numerical simulation to investigate the transport and electrochemical reaction phenomena, which can also be used to optimize the performance of fuel cell. In general, a trend of using numerical simulation to model PEMFC has developed, and it has become in complexity and accuracy as cheap computational power tool. The development of the PEMFC is generally quite costly and the use of mathematical modeling and simulations has become an important tool in the PEMFC development.

Most of the models are used to confirm effects studies of the parameter at different design parameters of fuel cell as like the operating parameters of pressure, temperature, the relative humidity of anode and cathode, the physical parameters of the GDE, porosity, conductivity etc. However the optimum combination of the parameters analysis of the PEMFC design is still lacking. To figure out the individual influence of every

Shan-Jen Cheng is with the School of Defense Science, Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan 33509, ROC. He is a Ph. D. candidate. (Corresponding author to provide phone: +886-3-3893475 fax: +886-3-3895924. e-mail: cheng5721@ gmail.com).

Jr-Ming Miao, is with Department of Materials Engineering, National PingTung University of Science & Technology, Shuefu Road, Neipu, Pingtung Taiwan.

Sheng-Ju Wu is with the Department of Power Vehicle and Systems Engineering, Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan 33509, ROC.

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parameter is not practical for integrating the system design. In this research the combination of all parameters were conducted to get the optimal design of the maximum power density in the PEMFC system. The statistical techniques have been widely applied to find out the optimal conditions for reducing the cost of the typical trial-and error approach. The statistical planned experiments of Taguchi's approach containing can reduce the required variations of parameters that must be studied for optimization design [9-11]. This approach provides a systematic and efficient method for optimizing a combination of numerous parameters. Therefore, this work presents the optimization of the maximum power density of performance by using Taguchi's method, and the performances are achieved by the simulation with CFD techniques. Finally, ANOVA is conducted to identify the critical parameters with respect to corresponding response.

II. PEMFC CFD MODEL AND TAGUCHI METHOD

A. PEMFC CFD model

Fig. 1 shows PEM fuel cell computational domain design with the parallel channel, consists of different zones from cathode to anode along the Z axis: current collectors, gas channels, gas diffuser layers, gas catalyst layers and a polymer membrane. Since we are studying the effect of operating parameters on the fuel cell performance, we have investigated many different conditions for the parameters. The reactants of anode and cathode flow fields are a counter –flow orientation. The flow flied pattern is closed to be the same as showed in ref. [12], and physical properties are summarized in Table I.

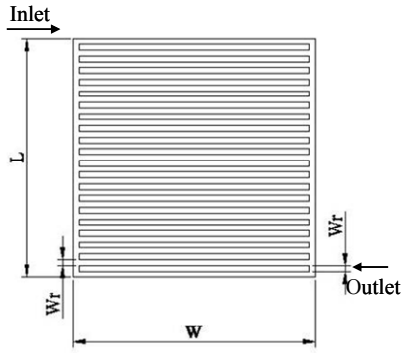


Fig. 1 PEMFC with parallel channel physical model

For optimal design and operating of PEMFC system, a detail and careful investigating of mass transport and electrochemical kinetics is essential. The proton exchange membrane of fuel cell is a complex physical coupling system of the complicated multiple electrochemical and transport phenomena. For investigated numerical three-dimensional fuel cell easily, on account of reduction computational time three-dimensional numerical model required some assumption is necessary. The model developed by commercial available CFD software Fluent6.3 code [13].

TABLE I
BASE PARAMETERS STUDIED FOR MODELING

Property	Values
Channel length (L)	50mm
Channel width (W)	1.2mm
Channel height (Wr)	1mm
Land area width	1.2mm
Gas diffusion thickness	0.2mm
Anode catalyst layer thickness	0.018mm
Cathode catalyst layer thickness	0.026mm
Membrane thickness	0.035mm
Electronic conductivity	$570Sm^{-1}$
Membrane permeability	$1.8\times10^{-18}\ m^2$
Diffusion and catalyst layers permeability	$1.76\times10^{-11}m^2$
Hydrogen exchange current density	$9.23\times10^{8}\ A/m^3$
Oxygen exchange current density	$1.05\times10^{6}\ A/m^3$
Diffusion and catalyst layers Porosity	0.4
Membrane porosity	0.28
Operating pressure	1atm
Anode transfer coefficient	0.5
Cathode transfer coefficient	1
Anode stoichiometric flow rate	2
Cathode stoichiometric flow rate	2
Relative humidity of anode	100%
Relative humidity of cathode	100%
Operating temperature	323k

The assumptions investigated in the three-dimensional models are followers: Operating is under steady-state and isothermal condition; The reactions are incompressible and laminar flow in the channel; Catalyst layers, porous electrodes and membrane are homogeneous and isotropic; Negligible contact resistance and gravitational field effect at the interface between the bipolar plates and the gas diffusion layers; Reactants and products are seen as continuous phase, so that Darcy's law is applied. The basic governing transport equations in the vector form are given as followed: The mass conservation also called continuity equation is giver by:

$$\frac{\partial(\rho v_x)}{\partial x}+\frac{\partial(\rho v_y)}{\partial y}+\frac{\partial(\rho v_z)}{\partial z}=0 \quad (1)$$

where ρ is the density of fluid, and v_i are the components of the velocity in x 、 y 、 z direction, respectively.

The momentum conservation also called as Navier-Stokes equation is given by:

$$\frac{\partial(\rho\varepsilon U)}{\partial t}+\nabla\cdot(\varepsilon\rho UU)=-\varepsilon\nabla p+\nabla\cdot(\varepsilon\mu\nabla U)+S_p \quad (2)$$

where U the fluid velocity vector; S_p is the source terms due to the pressure difference when a fluid passes through a porous medium. The source term is given by Darcy's law:

$$S_p=-\frac{\mu}{k}\varepsilon^2 U \quad (3)$$

where μ is the fluid viscosity in the medium; ε is the porosity of the medium; k is the permeability of the electrode

material and assumed to be constant.

In the fuel cell system of anode and cathode side, the inlet flow rates are showed as stoichiometric ratios of inlet streams based on a reference current density as followed:

$$u_{a,in} = \zeta_a \frac{I_{ref} A_{mem}}{2F} \frac{RT_{in}}{P_{a,in}} \frac{1}{X_{H_2}} \frac{1}{A_{ch}} \quad (4)$$

$$u_{c,in} = \zeta_c \frac{I_{ref} A_{mem}}{4F} \frac{RT_{in}}{P_{c,in}} \frac{1}{X_{O_2}} \frac{1}{A_{ch}} \quad (5)$$

where P_{in} is input gas pressure, T_{in} is operating temperature, A_{mem} the proton exchange membrane reaction area, A_{ch} Channel cross sectional area, X_i gas mole fraction of species, I_{ref} the reference average current density, ζ_i stoichiometric flow ratio velocities of anode or cathode sides.

B. Boundary condition

The boundary conditions were constrained for the model that was same for all the simulation cases studied. The operating temperature and pressure were constant. There are no-flux conditions everywhere besides the inlets and outlets of the flow channel. The inlet velocities of anode and cathode gas streams can be showed by their respective stoichiometric flow ratios, i.e., ζ_a and ζ_c fixed constant 2 and normal to the cross-section of the channel. At the outlets, velocity and species concentration fields are assumed fully developed for sufficiently long channels and no-slip boundary condition is used at the wall.

C. Numerical strategy

The model conservation equations were implemented by commercial CFD software Fluent6.3 code which using finite-volume method with KATIA as a preprocessor. Electrochemical Kinetics can be solved by user define functions (UDFs) capability and solution tactics is based on simple algorithm [14]. The velocity that the momentum equations solve was followed by solving continuity equation, which renews the pressure and flow rate. Results were then checked to be converged until the difference between successive iterations is less than 10^{-9} for all variables. As a grid test result showed, numerical investigated simulation model spatial resolution about 946,864 computational cells as shown in Fig. 2. At the HP-ML150 server computer, it is performed using the CFD code-Fluent6.3 about 7hr to computation of time for three-dimensional PEMFC numerical model.

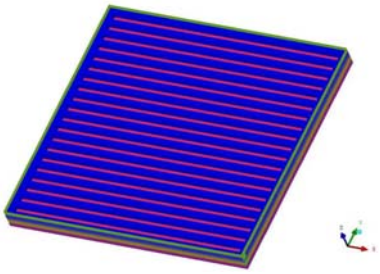


Fig. 2 PEMFC with parallel channel grid model

D. Taguchi method

General speaking, all possible combinations of the factor levels are considered by a factorial design approach. Due to the number of factors and levels increase, become extremely large experiment disadvantage. The Taguchi's orthogonal arrays (OAs) matrix method can be used to reduce the number of analyses runs. Taguchi method is a statistical method which was developed by Genichi Taguchi. It is a powerful tool of engineering for experimental optimization and one of the most well-known robust design methods. An approach of Taguchi method to find the optimum combination of the design factors to make the performance insensitive to the noise factors. The following steps of the Taguchi method involves:

(1)Analysis the problem and define objective function to be realized.

(2)Distinguish the design factors, levels and conduct the orthogonal arrays.

(3)Implement the experiment and analysis of performance dates.

(4)Recognize the optimal design factors and conform the quality characteristic.

(5)Complete the confirmation experiments for verification.

The Taguchi approach uses OAs from experimental design theory to analysis a large numbers of variables with a small number of experiments. An important of Taguchi method targets of factors design optimization are to build up the optimal combination and to minimize variations by resulting in target robust to the effect of noise.

E. Signal to noise(S/N) ratio

The Taguchi method gives the S/N ratio as the performance index to evaluate the quality characteristic of the product or process. It can be easily defined as the ratio of the mean (signal) to the standard deviation (noise) by S/N ratio. The quality characteristic can be optimized by S/N equation. The higher S/N ratio means a more consistent quality and a better system performance.

The S/N ratios may be depended on the particular type of quality characteristics, including lower-is-better (LB), higher-is-better (HB) or normal-is-best (NB). The objective function of the S/N ratio for the HB quality characteristics is in reference to the PEMFC performance of the maximum power density considered by

$$S/N(\eta) = -10 \times \log_{10}\left[\frac{1}{r}\sum_{i=1}^{r}\frac{1}{y_i^2}\right] \quad (6)$$

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Where r is number of tests in a trial (number of repetitions regardless of noise levels), y_i points out the measurement results, and subscript i indicates the number of simulation design factors arranged in the experiments of OA Table. The S/N response Table and response graph was constructed by S/N ratio, which then enabled the robust design effect of the factor to be applied.

F. Analysis of means (ANOM)

The statistical approach, analysis of means (ANOM), is used to determine the optimal combination of design factor. It is requisite to search the effects of each factor after computing the SN ratios in keeping with the experimental results. The effect of a factor level is defined as the deviation it causes from the overall mean. The effects of each factor can present the influence rank of each factor on quality characteristics and to find optimum combination of the factor levels from the response Table to response graph.

G. Statistical analysis of variance (ANOVA)

The percentage contribution indicates the relative power of a factor to reduce variation. The percentage contribution is a function of the sum of squares for each significant of fuel cell performance on quality characteristics. The F-test can be evaluated to consider factor significant affect the quality characteristics. The total variability data which measured by the total corrected to sum of squares and can be partitioned into a sum of squares of the differences both treatment averages and total average add to a sum of squares of the differences of observations within treatment from the treatment average [15].

III. Results and Discussions

A. Confirmation of the CFD results

In order to validate the results from numerical simulation model, the experimental data, type A flow channel, in [12] is compared the experimental and simulation results. The computed V-I polarization curve is presented in Fig. 3. Results calculated in good agreement with the experimental data and better than paper simulation data. Though in the single-phase, we neglect the effect of contact resistance and water flooding effect at the cathode side resulting in little over forecasted. The curve trend of current density still agreement well.

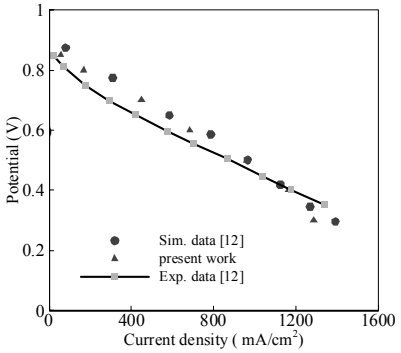


Fig. 3 Comparison of I-V curves between paper experimental and simulation data in [12]

B. Optimal design of Taguchi method

The design factors must think to have significant effects on the quality characteristic and can be set and maintained. The levels for each factor have to choose at this point. The number of levels for each factor identifies the experimental region. The orthogonal arrays from design of experiments theory were used by Dr. Taguchi to consider several variables with a small number of experiments. By means of OAs can greatly decrease the number of studied configurations. In this paper an $L_{18}(3^6)$ OA matrix was employed in the experiments matrix. The design factors and levels for the maximum power density are summarized in Table II. As shown, factors (A) pressure of fuel cell, (B) operating temperature, (C) the relative humidity of anode, (D) the relative humidity of cathode, (E) porosity of GDE, and (F) conductivity of GDE each have three levels range, respectively. A total of 18 CFD numerical simulations results I-V curves were conduction in Fig. 4.

TABLE II
DESIGN PARAMETERS AND LEVELS FOR MAXIMUM POWER DENSITY

Parameter	Units	Level 1	Level 2	Level 3
A	Pressure of fuel cell(atm)	1	2	3
B	Operating temperature(K)	60	70	80
C	The relative humidity of anode (%)	50	75	100
D	The relative humidity of cathode (%)	50	75	100
E	Porosity of GDE	0.4	0.5	0.6
F	conductivity of GDE(S/m)	200	570	1000

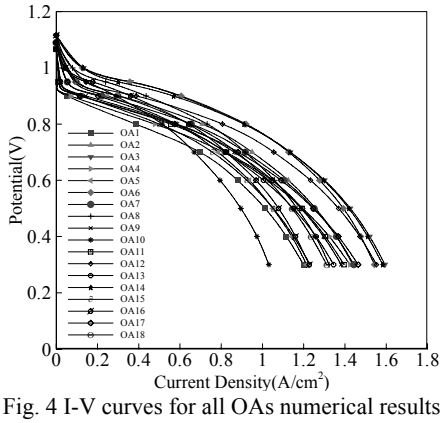


Fig. 4 I-V curves for all OAs numerical results

The maximum power density $L_{18}(3^6)$ is a HB characteristic. Eq. (6) is adopted to compute the S/N ratio values, which are presented in the last column of Table III.

TABLE III
S/N RATIO FOR MAXIMUM POWER DENSITY OF FUEL CELL

Tri.	A	B	C	D	E	F	Power-density (Mwatt/cm^2)	S/N (dB)
1	1	1	1	1	1	1	527.516	54.445
2	2	2	2	2	2	2	674.798	56.583
3	3	3	3	3	3	3	794.504	58.002
4	1	1	2	2	3	3	617.516	55.813
5	2	2	3	3	1	1	561.334	54.984
6	3	3	1	1	2	2	788.568	57.937
7	1	2	1	3	2	3	663.152	56.432
8	2	3	2	1	3	1	641.449	56.143

9	3	1	3	2	1	2	629.220	55.976
10	1	3	3	2	2	1	476.436	53.560
11	2	1	1	3	3	2	628.281	55.963
12	3	2	2	1	1	3	739.948	57.384
13	1	2	3	1	3	2	602.948	55.606
14	2	3	1	2	1	3	793.583	57.992
15	3	1	2	3	2	1	554.420	54.877
16	1	3	2	3	1	2	494.390	53.881
17	2	1	3	1	2	3	654.012	56.312
18	3	2	1	2	3	1	615.701	55.787

Based on the CFD data presented on the corresponding S/N response Table as shown in Table Ⅳ and S/N response graph can be obtain as shown Fig. 5. In accordance with the principles of the Taguchi method, the present study assumes that the highest product quality is indicated by the maximum S/N ratio.

TABLE Ⅳ
S/N RESPONSE TABLE FOR MAXIMUM POWER DENSITY

Factors	Levels			Main effects
	1	2	3	
A	55.956	56.33	56.66	1.704
B	55.564	56.13	56.253	0.688
C	56.426	55.78	55.74	0.686
D	56.304	55.952	55.69	0.614
E	55.777	55.95	56.219	0.442
F	54.777	55.991	56.989	2.023

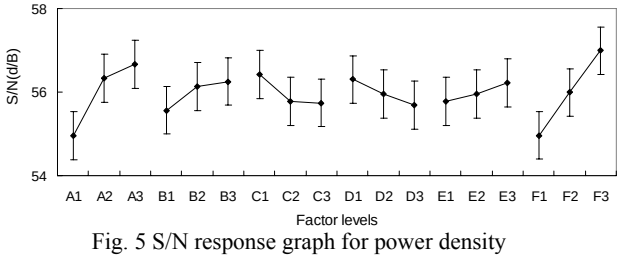


Fig. 5 S/N response graph for power density

Typical parameter analysis trends to focus on the effect result from the variation of a single parameter only. Therefore, the statistical technique is an attractive approach because it can save more time and resource than the traditional trial-and-error analysis.

Before processing the statistical analysis, Table V summarizes the ANOVA results for maximum power density. The percentage contribution and variance of factors F, A, B, and C rank that the conductivity of GDE, pressure of fuel cell, the relative humidity of anode and operating temperature are influential design factors. Conversely, the result indicate that the relative humidity of cathode and porosity of GDE design factors have a small sum of squares pooled as error and a less significant influent upon the maximum power density in our case study.

TABLE V
ANOVA OF THE OPTIMAL DESIGN FOR MAXIMUM POWER DENSITY

Factor	SS	DOF	MS	F	Contribution (%)
A	9.801	2	4.901	10.508	29.888
B	1.617	2	0.809	1.734	2.306
C	1.778	2	0.889	1.907	2.850
D	1.141			Pooling	
E	0.595			Pooling	
F	12.278	2	6.139	13.164	38.237
Error	2.462	5			
Pooled Error	4.197	9	0.466		26.719
Total	29.672	17			100

Note: Factors D, E are pooled as error due to a small sum of squares.

Therefore, as presented in Fig. 5 reveals the optimal design parameter combination, A3B3C1D1E3F3, and the corresponding value of each factor for the maximum power density, i.e. A3: pressure of fuel cell (3atm); B3: operating temperature (353K); C1: the relative humidity of anode (50%); D1: the relative humidity of cathode (50%); E3: porosity of GDE (0.6); F3: conductivity of GDE (1000S/m).

In order to prevent an over-estimate, factor D and E are not considered and the estimated S/N ratio η_{opt} is computed as:

$$\eta_{opt} = (\eta_{A3} + \eta_{B3} + \eta_{C1} + \eta_{F3}) - (3\overline{\eta}) \\ = 58.382\ (dB) \quad (7)$$

The final step is to determine the estimated value with the confirmative experimental value, using the optimal levels of the control factors to confirm experimental reproducibility.

A confidence interval (CI) is a range between the maximum and minimum values. The true average has some stated percentage of confidence. The confidence limits on the above estimated can be calculated using the following equation:

$$CI = \sqrt{F_{\alpha,v_1,v_2} V_{ep} (\frac{1}{n_{eff}} + \frac{1}{r})} \quad (8)$$

where F_{α,v_1,v_2} is the F-ratio required for ($\alpha = 0.05$ with a confidence of 95%); $v_1$is the number of degree of freedom of the mean; v_2 is the number of degree freedom of the error; V_{ep} is the error of variance; r is the sample size in the confirmation experiment, and neff is the effective sample size.

$$n_{eff} = \frac{N}{1 + DOF_{opt}} \quad (9)$$

Where N is total number of trials and DOF_{opt} is the total degrees of freedom that are associated with items used to estimate η_{opt} .Given a CI of 95% for the maximum power density, Vep=0.466, the sample size in the confirmation experimentation r is 1, N is 18, DOF_{opt} is 8, and the effective sample size n_{eff} is 2. Therefore, the CI is computed to be CI=1.73. In the demonstration study, the confirmation test result was showed that the new maximum power density, $P_{\max}$, was 818.7324, with a S/N ratio value of 58.263. These values represent an improvement over the original results, and hence this verification exercise enhances confidence in the technique.

As the analysis results in Table Ⅵ and Fig. 6 shown in, Taguchi method can employ the optimum robust combination among the design parameters.

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TABLE VI
COMPARISON BETWEEN INITIAL AND OPTIMUM PARAMETER OF TAGUCHI S/N RATIO

Tri..	Combination factors	Power-density (Mw/cm^2)	S/N (dB)
Original-max (OA3)	A3B3C3D3E3F3	794.504	58.002
Optimum	A3B3C1D1E3F3	818.732	58.263

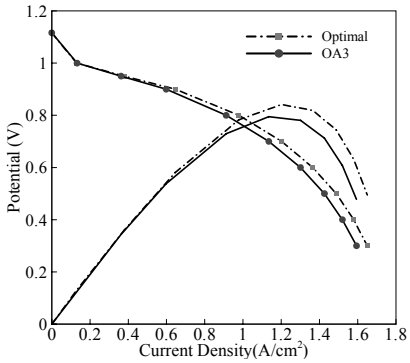
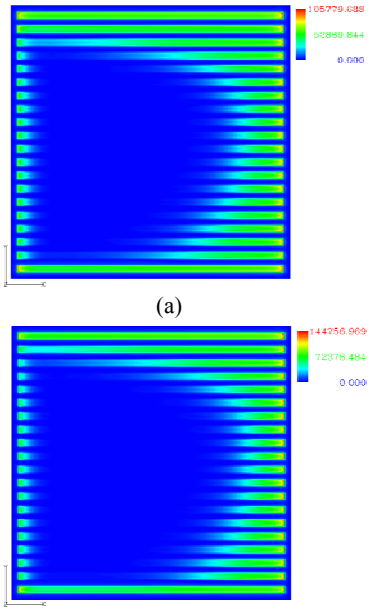


Fig. 6 Comparisons of I-V curves between original (OA3) and optimum results

Fig. 7 illustrates the local current density in collector of the PEMFC performance for optimum combination condition better than original result.

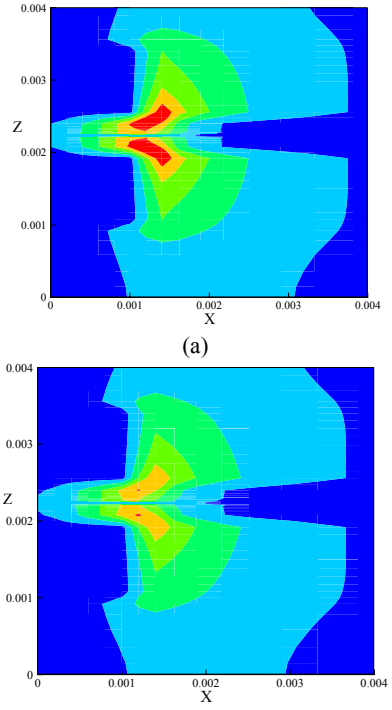


(a)

(b)

Fig. 7 Local current density in the collector
(a) OA3 (b) Optimum

As shown in Fig. 8, a lower porosity value has a larger total current fraction than higher porosity value in the channel area. That can lead to local hot-spots and dry out within membrane. The performance decreased since the electric resistance increasing and more heat generate which lead to membrane failure. The current density keep relatively even through the cell is important.



(a)

(b)

Fig. 8 Local current density in cathode catalyst layer
(a) OA3-porosity=0.6(b) Optim-porosity=0.4

IV. CONCLUSION AND FUTURE RESEARCHES

In this paper, an integrated CFD and Taguchi method to optimize the operating condition for maximum power density of PEMFC performance. The effects of porosity of GDE and local current density on the fuel cell performance can be checked by CFD calculation with I-V curve and contour plots Based on this research in the present show can be drawn from CFD computation as follow:

(1)Taguchi method can be used to investigate the effect of performance for PEMFC. The degree of ANOM parameters on maximum power density are: conductivity of GDE, pressure of fuel cell, operating temperature, the relative of humidity of anode, besides the relative humidity of cathode and porosity of GDE are pooled as error due to a small sum of squares.

(2)The optimum combination conditions that are pressure of fuel cell 3 atm, operating temperature 353K, the relative humidity of anode 50% and cathode 50%, porosity of GDE 0.6, conductivity of GDE 1000 from ANOVA and confirm interval test obtained maximum power density through comparison with the original result, the PEMFC performance is improved after optimization.

(3)The show approach can be realize by combining a multi-physics model for PEMFC parameters with CFD calculation and provide a tool for applying to fuel cell stacks with performance in the future.

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