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PARAMETRIC ANALYSIS OF PROTON EXCHANGE MEMBRANE FUEL CELL (PEMFC) PERFORMED BY THE TAGUCHI METHOD

Summary

The proton exchange membrane fuel cell (PEMFC) performance depends on the design parameters like landing-to-channel width ratio (L:C), channel depth, shape and number of passes on the flow channel, and operating parameters like temperature, pressure, the stoichiometric ratio of reactants, relative humidity, back pressure on the anode, and cathode flow channels. In this paper, optimization of design and operating parameters such as various landing -to-channel width ratios (L:C -1:1, 1:2, 2:1, and 2:2) of the interdigitated flow channel, pressure, temperature, and the anode and cathode inlet reactant masses on the 25cm^2 electrode surface active area of the PEMFC was carried out. A three dimensional (3-D) PEMFC model was created by Creo Parametric 1.0, meshed by ICEM 14.0 and simulated using the CFD Fluent 14.0 software packages. The optimization of the design and operating parameters was carried out in two stages using Minitab 17 with a standard orthogonal array of the Taguchi method. From the first stage of analysis, it was inferred that the landing-to-channel width ratio (L:C - 1:1) has the biggest influence on the PEMFC performance and the square of response factor (R^2) was achieved by the Taguchi method at 97.95%. In the second stage of analysis, fine-tuned optimization was performed on selected factors which cause an increase in power density of 0.81. Also, R^2 was achieved at 100 % and the results were also validated using the CFD Fluent 14.0 software packages.

Key words: *Optimization; Operating parameters; Design parameters; 3-D PEMFC Model; Taguchi method.*

1. Introduction

The PEMFC is an environmentally friendly power source which is suitable for powering both portable devices and mobile application due to their high energy density and lower operating temperature range [1]. The PEMFC consists of a solid polymer electrolyte membrane (Nafion) placed between two electrodes, the anode and the cathode. The electrochemical reaction produces electricity along with water and heat as byproducts. Standard physical conservation equations, such as mass, momentum, charge and energy equations have been considered. Various flow channel designs have been used to obtain high current and peak power density, proper temperature distribution, and optimum water management. The influence of the flow channel path length on the PEMFC flow field design

was addressed by Shimpalee et al. [2]. However, water is a by-product of the electrochemical reaction on the cathode flow channel and the partial pressure of water vapour causes condensation of water on the anode flow channel. Therefore, the water management of a PEMFC has become an important task since too much accumulated water causes "flooding" and insufficient amount of accumulated water causes dryness of the membrane and can adversely affect the performance and lifetime of PEMFCs. Water flooding will make the PEM fuel cell performance unpredictable and unreliable under the nominally identical operating conditions. This critical issue related to PEMFCs can be dealt with through the appropriate design of flow channels for the effective removal of water built on the flow field (bipolar) plates. In order to enhance the performance and reliability of PEMFCs, it is important to know more about the mechanism which causes the performance loss, such as non-uniform concentration, current density distributions, high ionic resistance due to a dry membrane and high diffusive resistance due to the flooding on the cathode, which was addressed by Nattawut Jaruwasupant &Yottana Khunatorn [3] and Owejan et al. [4]. Hydration of the membrane is essential for maintaining the performance of PEMFCs. If hydration is not maintained properly, flooding and dehydration will occur, which affects the fuel cell performance [5, 6]. Identifying the proper flow channel and the flow field design is also of importance as they also affect the performance of the fuel cell significantly [7].

However, operating parameters like pressure, temperature, and reactants influence the performance of PEMFCs considerably. Increasing the inlet pressure improves the consumption of reactants and results in more homogeneous distribution. The straight channel design also affects the consumption of reactants and consequently results in an increase in water production [8]. It is clearly evident that there is an urgent need for analyzing the simultaneous influence of operating and design parameters on the performance of the PEMFC. It was done in our study by using the CFD Fluent 14.0 software packages and the Taguchi method using MINITAB 17. This paper gives a detailed study on the optimization of various landing-to-channel width ratios (L:C - 1:1,1:2, 2:1, and 2:2) of the interdigitated flow channel and operating parameters such as pressure, temperature, the anode and the cathode inlet reactant mass of the 25 cm^2 electrode surface active area of PEMFC and the influences of their performance were compared. Karthikeyan et al. [9] optimized ten operating and design parameters of a single channelled PEMFC using the Taguchi method. The maximum power density corresponding to Taguchi calculations was in good agreement with the results obtained by the data analysis software, indicating that the Taguchi method is suitable for PEMFC applications [10].

2. Model development

A three dimensional (3-D) PEMFC model with an interdigitated flow channel of various landing-to-channel width configurations was developed by Creo Parametric 1.0, as shown in Fig.1. The modelling was done by creating individual parts of the PEMFC such as the anode and the cathode, the gas diffusion layer (GDL), the solid polymer electrolyte (Nafion) membrane, the anode and cathode catalyst layers.

Table 1 Dimensions and zone type of the fuel cell parts

S.No	Part Name	Width (mm)	Length (mm)	Thickness (mm)	Zone type
1	Anode and the cathode flow channel	80	80	10	Solid
2	Anode and the cathode catalyst	50	50	0.08	Fluid
3	Membrane	50	50	0.127	Fluid
4	GDL anode and cathode	50	50	0.3	Fluid

These parts were assembled using suitable constraints to form a 3-D PEMFC. The assignments of zones for various parts were done by Workbench 14.0. The dimensions, the names of the components and the zone type are given in Table 1. Various geometric models (landing-to-channel width ratios of 1:1, 1:2, 2:1, and 2:2) of the interdigitated flow channel were meshed by using ICEM 14.0 (a module of Ansys 14.0).

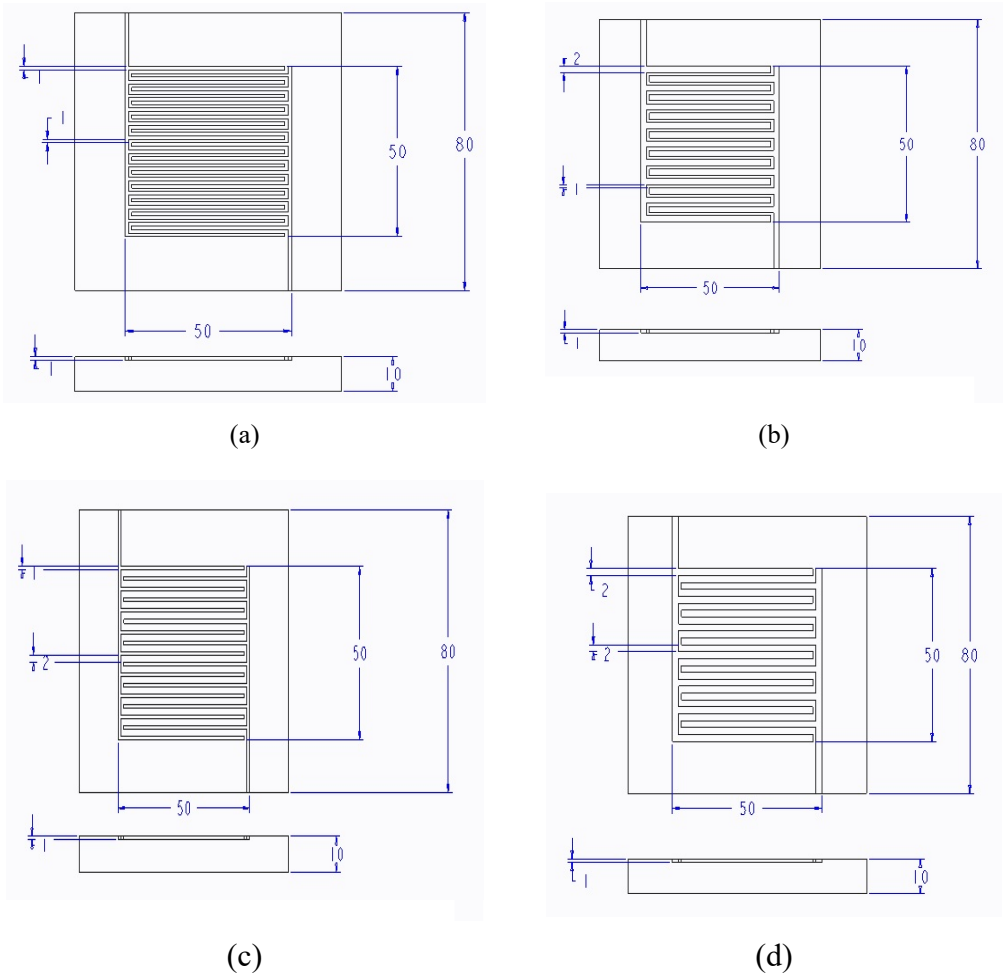

Fig. 1 Various landing-to-channel width ratios (L: C) (a) 1:1 (b) 1:2 (c) 2:1, and (d) 2:2 of the interdigitated flow channel of 25 cm^2 active area.

2.1 Governing Equations

The simulation has been solved by simultaneous equations like conservation of mass, momentum, energy, species concentration, butler–Volmer equation, Joule heating reaction, and the Nernst equation to obtain reaction kinetics of the PEMFC. The model was used to consider the system as three-dimensional and steady, the inlet gases as ideal, the system as isothermal, the flow as laminar, the fluid as incompressible, the thermo physical properties as constant, and the porous GDL, both catalyst layers and the membrane, as isotropic. Creating a good mesh has been one of the most difficult steps involved in the modelling. A careful balance is required in creating enough computational cells to capture the geometry without creating too many of them. Care should be taken so that their number would not exceed the available memory of the meshing computer. Many other factors must also be taken into account in order to generate a computational mesh which provides representative results when simulated [11].

2.2 Meshing on PEMFC

After geometry building, the next step was discretization, which was done by the ANSYS 14 ICEM software. The entire cell was divided into a finite number of discrete volume elements or computational cells to solve the equations associated with the fuel cell simulation. Blocking was done using the split block method and meshing was done using the Cartesian method. Body fitted mesh was used and projection factor was set to 1. The projection factor determines how closely the edges of the mesh match up with the grid. The meshing method was used as a Cartesian grid, which helped to form the hexahedral mesh to get accurate results, as shown in Fig.2. For all the models, a minimum of 557667and a maximum of 561990 nodes, a minimum of 723512 and a maximum of 734568 elements have been considered in our studies

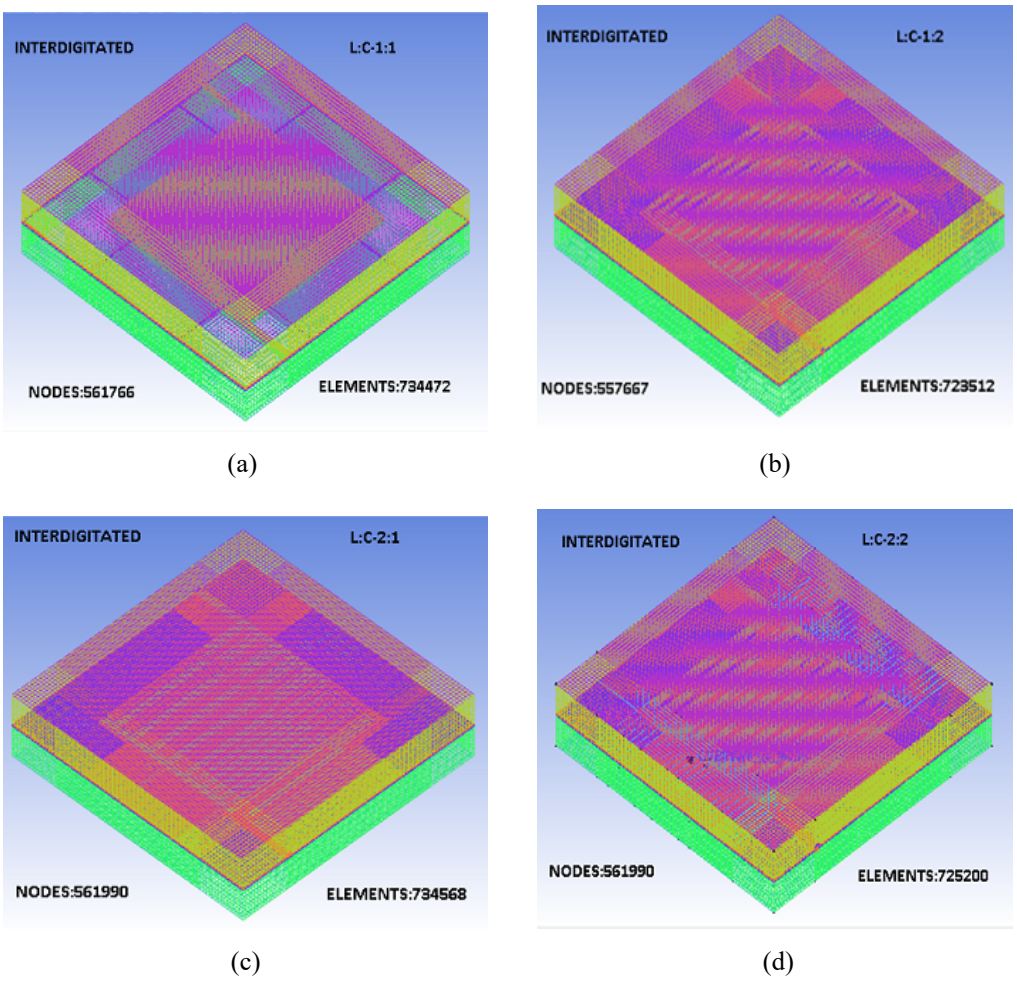

Fig. 2 Meshed assemblies of interdigitated flow channel using ICEM

2.3 Solver

A finite volume approach based on the commercial solver FLUENT 14.0 was used to solve the various governing equations. The 3D, the double precision and the serial processing were used for this model. The species concentration on the anode side of H_2, O_2, and H_2O were 0.8, 0, and 0.2, respectively. Similarly, on the cathode side, they were 0, 0.2, and 0.1, respectively. Open circuit voltage was set at 0.95 V. The anode was grounded and the cathode voltage was varied from 0.05 V to 0.95 V for solving the reaction kinetics in order to get the current flux density, H_2, O_2, and H_2O fractions along with the flow field design. Multigrid settings were modified as F-Cycle for all equations and the entered termination restriction

value was set as 0.001 for H_2, O_2, H_2O, and water saturation. The electric and proton potential values were set at 0.0001. The stabilized version of the biconjugate gradient method (Krylov-space method) BCGSTAB was selected for H_2, O_2, H_2O, water saturation, and electric and proton potential.

3. Adaptation of the Taguchi method

The Taguchi method can be used to reduce the number of experiments to a practically feasible level without any sacrifice in considering any factor or even any one of its levels. Hence, this method can also be used to find out the optimum combination among the input parameters which will result in getting the maximum possible output which in turn results in the enhanced performance of the PEMFC. In this analysis, the Taguchi method L16 standard orthogonal array with a 4-level design and a maximum of 5 factors was used and to find the significance of these factors where low, middle, and high range values were considered. When the orthogonal array was used, the significance of factors and the optimum combination would be found during 16 runs. The analysis was performed in two stages, namely, in the coarse optimization of factors and in the refinement of coarsely optimized factors. The theoretical value of hydrogen on the anode side was 4.33E-07 kg/sec and on the cathode side it was 3.33E-06 kg/sec. The anode and cathode inlet mass flow rates of the reactants given as 3, 3.5, 4, and 4.5 (the given numerical values show the number of times by which the theoretical mass flow rate has to be multiplied).

4. Results and Discussion

Table 2 Power density and S/N ratio for 16 runs

Run	L:C	Pressure (bar)	Temperature (K)	Hydrogen mass flow rate (kg/s)	Oxygen mass flow rate (kg/s)	Power density (W/cm^2)	S/N ratio
1	1:1	1	323	3	3	0.302	-10.410
2		1.5	333	3.5	3.5	0.332	-9.572
3		2	343	4	4	0.362	-8.818
4		2.5	353	4.5	4.5	0.357	-8.941
5	1:2	1	333	4	4.5	0.304	-10.345
6		1.5	323	4.5	4	0.311	-10.133
7		2	353	3	3.5	0.299	-10.477
8		2.5	343	3.5	3	0.373	-8.577
9	2:1	1	343	4.5	3.5	0.270	-11.368
10		1.5	353	4	3	0.254	-11.887
11		2	323	3.5	4.5	0.314	-10.055
12		2.5	333	3	4	0.338	-9.420
13	2:2	1	353	3.5	4	0.266	-11.493
14		1.5	343	3	4.5	0.295	-10.603
15		2	333	4.5	3	0.311	-10.145
16		2.5	323	4	3.5	0.344	-9.264
Overall mean S/N ratio							-10.094

The combinations of these levels were derived using the MINITAB 17 software for the standard L16 orthogonal array. As per L16 orthogonal array, the inputs were given to the analysis software and all other parameters were constant. The power density from the polarization curve was found by a numerical study using the CFD Fluent 14.0 software packages for all 16 runs and the corresponding Signal/Noise (S/N) ratios shown in Table 2 were found using the MINITAB 17 software. The S/N ratio, i.e. the ratio between the controlled and uncontrolled factors, was calculated using the formula -10 log10 ($1/P^2$), where P is the power density.

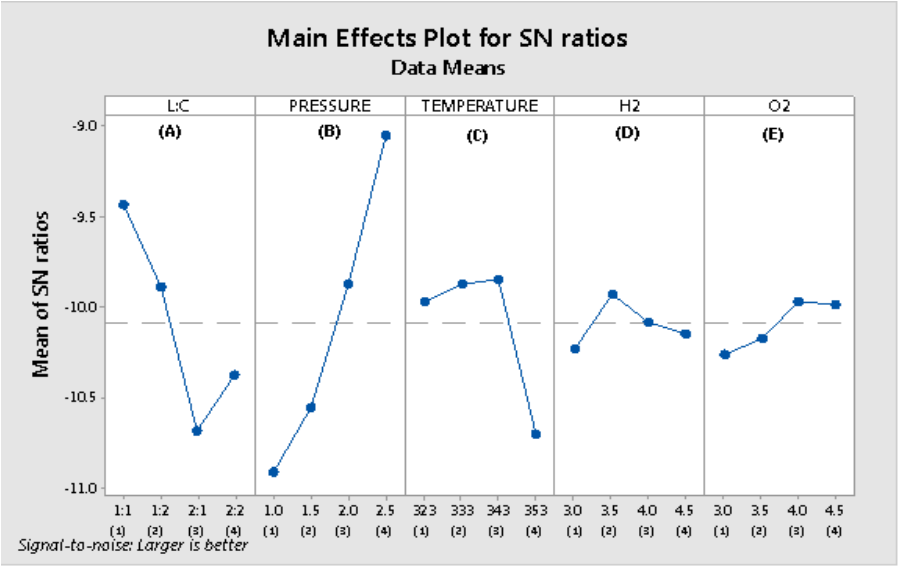

Fig. 3 Mean S/N ratio plot for L: C (A), Pressure (B), Temperature (C), H_2 (D) and O_2 (E)

The maximum S/N ratio gives better performance, according to the analysis based on "Larger the better" and the optimum combination of operating and design parameters was found to be A1B4C3D2E3 (as shown in Figure 3). It was concluded that the landing-to-channel width ratio of interdigitated flow channel of 1:1 (A1) and the operating parameters such as pressure of 2.5 bar (B4), temperature of 343 K (C3), theoretical consumption of hydrogen and oxygen of 3.5 (D2) and 4.0 (E3), respectively, were the optimum parameters for obtaining a better performance of the PEMFC.

Table 3 Mean S/N ratios, Delta, and Rank for each level of factors

Factors	Level 1	Level 2	Level 3	Level 4	Delta	Rank
Landing-to-channel width (L:C)	-9.435	-9.883	-10.682	-10.376	1.247	2
Pressure /bar	-10.904	-10.549	-9.873	-9.05	1.854	1
Temperature /K	-9.965	-9.871	-9.841	-10.699	0.858	3
Hydrogen mass flow rate / kg/s	-10.228	-9.924	-10.078	-10.146	0.303	4
Oxygen mass flow rate / kg/s	-10.255	-10.17	-9.966	-9.986	0.289	5

The optimization was performed in the larger the better type of Taguchi method for the power output of the PEMFC to be maximized. The optimization results of various parameters were based on S/N ratios and the significance of each factor was determined by ranking them according to their performance. The Delta value of each factor available in the MINITAB 17 software is shown in Table 3. The factor with the highest delta value indicates greater significance. It was found that pressure was the predominant factor affecting the performance

of a fuel cell. The other parameters influencing the output of the PEMFC to a considerable extent are the landing-to-channel width ratio (L: C) of interdigitated flow channel design, temperature, and the consumption of hydrogen and oxygen mass flows.

4.1 Optimization of design and operating parameters

Generally, the factors which have a less significant effect on the response would be neglected in further analysis, but in this analysis, all the factors were considered irrespective of their significance related to a better performance of the PEMFC. The maximum power density of this combination found using the Taguchi calculation was 0.4055 W/cm², as shown by equation (1).

S/N ratio for the optimum combination

$$\eta_{opt} = \eta+\Delta A1+\Delta B4+\Delta C3+\Delta D2+\Delta E3=-10\log10(1/P_{max}^2) \quad (1)$$

$$\eta_{opt} = -10.094 + (0.659+1.044+0.253+0.170+0.128) = -7.840 = -10\log10\,(1/P_{max}^2)$$

$$P_{max} = 0.4055 W/cm^2$$

(ΔA1 corresponds to the difference between the overall S/N ratio mean and the maximum value of S/N ratio mean for all the four levels corresponding to the factor A (10.094-9.435=0.659); ΔB4 corresponds to the difference between the overall S/N ratio mean and the maximum value of S/N ratio mean for all the four levels corresponding to the factor B (10.094-9.05=1.044) in Table 3, and so on; η corresponds to the overall mean of the S/N ratio in Table 2).

In order to validate the power density obtained by the Taguchi method, the optimum combination of parameters was given as input to the CFD Fluent 14.0 software package for a cell potential of 0.5 V and the current density of 0.815 A/cm^2. The maximum peak power density was found to be 0.4075 W/cm² on the 25cm^2 PEMFC performance. This was in good agreement with the power density obtained from the Taguchi calculation with a deviation percentage of 0.493 and the square of response factor (R^2) of 97.95% achieved and computed by the MINITAB 17 software. Thus, the methodology developed in this research proves that the PEMFC gives the best performance when operated at a pressure of 2.5 bar, operating temperature of 343 K, landing-to-channel width ratio of interdigitated flow channel of 1:1, and hydrogen and oxygen mass flow rates 3.5 and 4.0 times the theoretical mass flow rates.

4.2 Refinement of coarsely optimized parameters

The optimum values of operating and design parameters were found from the first stage of optimization. The second stage of the Taguchi analysis was performed for three parameters with the standard L9 orthogonal array with three different levels to find accurate values. Even though the landing-to-channel width ratio was classified as a second rank in the first stage of optimization, it was not considered due to the difficulties in the machining of flow channels with dimensions lower than 1:1. Therefore, the pressure, the temperature and the hydrogen mass flow rate were only considered in the second stage of optimization with a common landing-to-channel width ratio of 1:1. These levels were chosen to be close to the optimum levels found in the first stage in order to refine them further. Thus, nine combinations based on the standard L9 orthogonal array were given as input to the MINITAB 17 software and the corresponding values of power density were found by the CFD Fluent 14.0 software packages for all 9 runs. The power density and the S/N ratio values are shown in Table 4.

Table 4 Power density and S/N ratio of fine-tuned parameters for 9 runs

Run	L:C	Pressure (Bar)	Temperature (K)	Hydrogen mass flow rate (kg/s)	Power density (W/cm^2)	S/N ratio
1	1.1	2.5	338	3.25	0.335	-9.503
2			343	3.5	0.336	-9.468
3			348	3.75	0.361	-8.842
4	1.1	2.75	338	3.5	0.330	-9.627
5			343	3.75	0.354	-9.026
6			348	3.25	0.347	-9.198
7	1.1	3	338	3.75	0.338	-9.412
8			343	3.25	0.359	-8.890
9			348	3.5	0.428	-7.377
Overall Mean S/N Ratio						-9.038

Fig.4 shows plots of refined parameters for the S/N ratio generated by the MINITAB 17. It was found that A3B3C2 was the optimum level with the highest S/N ratio. Thus, the refined optimized parameters were found to be as follows: pressure of 3 bar, cell temperature of 348 K, and anode hydrogen mass flow rate of 3.5 times the theoretical mass flow rate.

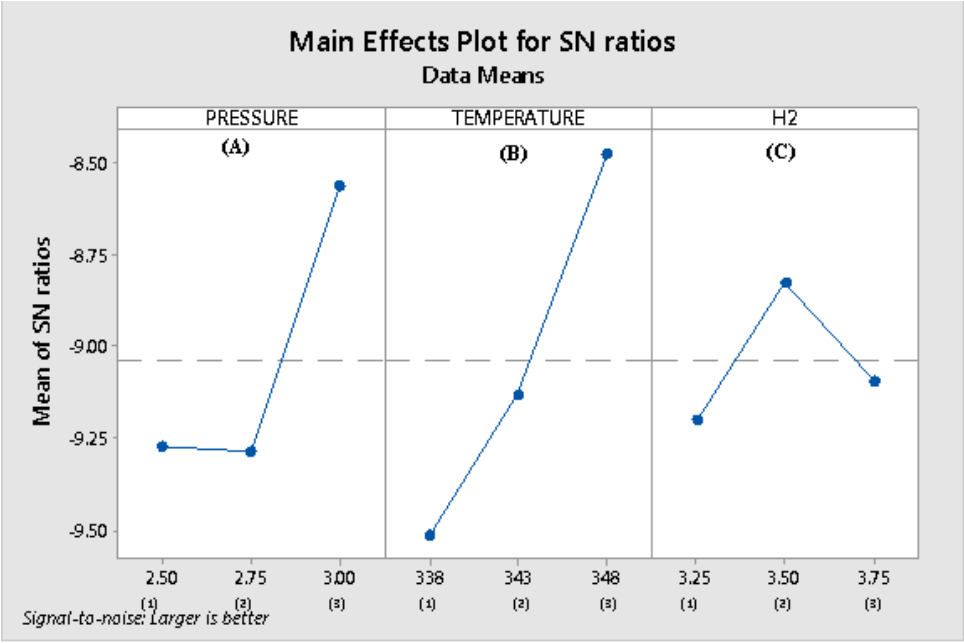

Fig. 4 Mean S/N ratio plot for refined parameters of Pressure (A), Temperature (B) and H_2 (C)

As per the calculations of the equation (1), the maximum power density for this optimum combination was found to be 0.408 W/cm². The Delta value and the rank of all three factors were generated by the MINITAB 17 software and the corresponding values are given in Table 5. When the refined optimum combination of the three factors was given to the CFD software as input, the maximum power was found to be 0.4086 W/cm². The deviation in result was 0.147% and R^2 was achieved at 100%.

Table 5 Delta value and rank for the second stage of analysis

Factor	Level 1	Level 2	Level 3	Delta	Rank
Pressure / bar	-9.271	-9.284	-8.56	0.724	2
Temperature / K	-9.514	-9.128	-8.472	1.041	1
Hydrogen mass flow rate / kg/s	-9.197	-8.824	-9.093	0.373	3

It is proved that by increasing the number of levels through the usage of two-stage optimization the error is getting reduced. Hence, it means that the model generates more accurate results. Thus, the refined optimized combination of input parameters was found to be the pressure of 3 bar and the cell temperature of 348 K.

5. Conclusion

The maximum power density for optimized parameters of PEMFC obtained by using Minitab 17 was 0.406 W/cm^2 and from the CFD model it was 0.408 W/cm^2. Obviously, the power density increased by 0.493 % and the R^2 value obtained in the first level of optimization was 97.95%. In the fine refinement stage, the values of 0.408 W/cm^2 and 0.4086 W/cm^2 of power density were achieved by the Taguchi method and the CFD model respectively, with an increment in power density of 0.147 % at 100 percentage of R^2 value. The effect of design and operating parameters on the performance of PEMFC was more significant. The maximum power density corresponding to Taguchi calculations was in good agreement with the software results, indicating the suitability of the Taguchi method for PEMFC applications.

Nomenclature

H - overall mean S/N ratio
η_{opt} - mean corresponding to the optimum combination
Δ - difference of values
P_{max} - maximum power density (W/cm^2)

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