



Response Surface Methodology Approach for Modeling and Performance Optimization of PEM Fuel Cells

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Abstract: Polymer Electrolyte Membrane (PEM) fuel cells are a popular green source of electrical energy and is often used in applications like electric vehicles due to its environmentally friendly operation. This type of fuel cell has a low operating temperature, light weight, and negligible emission of greenhouse gases. However, the PEM fuel cell is a complex multivariable system with a large number of input and output factors, and most of the input factors affect output factors directly or indirectly. As a result, it is conventionally quite difficult to determine which input factor has a major effect on a particular output factor. Statistical methods are very popular for finding the individual and interaction effects of input factors on output factors. In this paper, for the first time, a simple and realistic MATLAB SIMULINK model for a PEM fuel cell is presented to conduct various experimental tests. The developed MATLAB SIMULINK model and statistical design of experiments, Response Surface Methodology (RSM), are used to develop metamodels (mathematical models of the simulation model) for the PEM fuel cell to find the individual and interaction effects of various input factors on output factors. The developed metamodels can be used to find the region for optimum operation of the presented fuel cell. The metamodels are validated by conducting four different statistical tests. The optimum point of operation is presented by calculating stationary points from the metamodels.

Keywords: SIMULINK Model; Metamodel; Counter plots; Response surface

Introduction

Fuel cells are very popular as a green energy source of electrical energy, as the hazardous green house gases emitted during energy conversion process in all types of fuel cells are negligible and hence energy conversion is considered to be environment friendly. Fuel cells are generally classified according to electrolyte used and operating temperatures. The PEM fuel cell is a low temperature fuel cell mostly demanded in electric mobility applications due to its simple structure, quick start, high power density, low operating temperature and negligible environmental effects [1][2]. For modeling and analysis of complex systems, the statistical design of experiment response surface methodology, which is a simple and user friendly mathematical tool, can be used to express output factors in terms of input factors with

optimized response. The objective of the response surface methodology is to understand the topology of response surface and find the region where the optimal response occurs [3] [4].

As the demand on PEM fuel cells increases, numbers of mathematical models have been reported in literature to represent its static and dynamic behavior. In this paper, a simple but accurate SIMULINK model of PEM fuel cell is developed for performance analysis. The presented simulation model is a generalized model and thus applicable to PEM fuel cells of any rating. Using test data obtained from the SIMULINK model and statistical experiments, first and second order Metamodels are developed for PEM fuel cell which can be used to find individual or interaction effects of input factors on output factors. The validation of Metamodels is also presented.



Development of the PEM Fuel Cell SIMULINK Model

To analyze the operating performance of PEM fuel cells, numbers of mathematical models, static as well as dynamic, have been reported in literature [5][6][7][8][9][10][11][12]. The previous models in literature are either very complex or require a huge amount of experimental data for modeling and simulation. The proposed models in this paper are simple, optimized and more realistic without requiring as much experimental data compared to the previous models to create. The details of the developed Simulink model have been presented in the authors' previous research [13].

The developed MATLAB SIMULINK model of a PEM fuel cell is shown in Fig. 1. This simulation model consists of several sub-models to establish the relationships between various input and output factors. The simulation model was previously validated using practical PEM fuel cells developed by the author in [13]. The SIMULINK model has been validated against practical PEM fuel cells under the same environmental conditions. This model allows for the analysis of the effects of one or more input factors on one or more output factors.

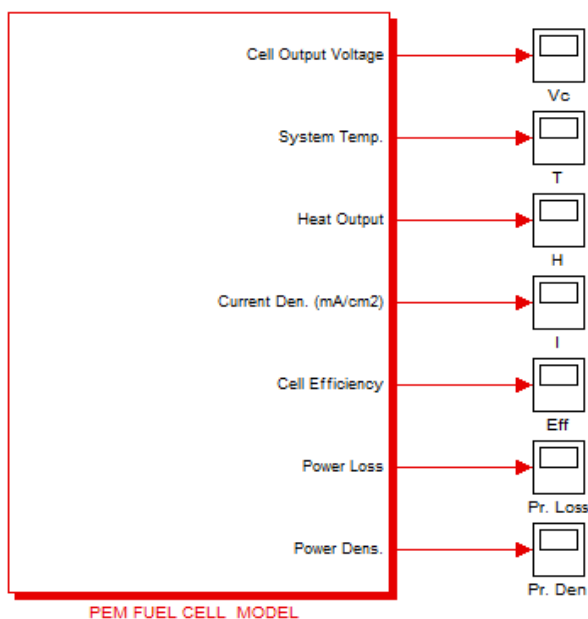


Fig. 1. Main Model of PEM fuel cell

Development of Metamodels

The Metamodel is a mathematical model developed using principle of statistical modeling and MATLAB SIMULINK model. Many experiments to develop the Metamodels were conducted using the simulation models. One such experiment involved changing input factors to

better understand the input/output relationship.

The development of first order model and selection of input factor levels

The terminal voltage of a PEM fuel cell is influenced by various polarizations and decreases as the current drawn from the fuel cell increases while optimum performance of a PEM fuel cell is achievable when it operates in the high power density region. [14]. To develop Metamodels, the controllable input factors used for analysis are fuel cell current (I), mass flow rate of hydrogen (H) and cell internal capacitance (C) whereas the output factors considered for analysis are cell output voltage (V) and cell power density (P). The response factors are the functions of input factors and hence they are changing with respect to change in any input factor.

The first step in the proposed statistical response surface methodology is to select ranges of input factors. Here the selected input factors are coded into variable x_1 , x_2 and x_3 respectively. Table 1 shows ranges of input factors selected for analysis.

Table 1. Selection of input factors

Input Factor	Input variables	Highest value	Lowest value	Base value
Fuel cell current (mA/cm ²)	x_1	150	450	300
Mass flow rate of Hydrogen (SLPM)	x_2	0.1	0.5	0.3
Cell Internal Capacitance (F/g)	x_3	50	250	150

Development and Analysis of First Order Model

In first order Metamodel, the approximated function has linear relation with independent variables. This model can effectively be represented as,

$$y_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \dots + \theta_q x_{iq} + e \quad (1)$$

where, y is response function, $x_1, x_2 \dots x_i$ as design variables, β_j 's regression coefficients and e as a statistical error term.

The first order Metamodels are very effective to represent flat surfaces [15]. To develop this model, a single replicate $2^3=8$ experimental test was conducted on simulation model and the results of these eight runs are shown in Table 2.



Table 2. Data for processing first order model

Input Factors			Coded Factors			Responses	
<i>I</i>	<i>H</i>	<i>C</i>	x_1	x_2	x_3	<i>V</i> (V)	<i>P</i> (W//cm ²)
150	0.1	50	-1	-1	-1	0.73	0.10
450	0.1	50	1	-1	-1	0.62	0.27
150	0.5	50	-1	1	-1	0.75	0.11
450	0.5	50	1	1	-1	0.64	0.28
150	0.1	250	-1	-1	1	1.10	0.18
450	0.1	250	1	-1	1	0.92	0.42
150	0.5	250	-1	1	1	1.21	0.45
450	0.5	250	1	1	1	1.16	0.55

All input factors are coded in the interval -1 to +1. The zero (0) indicate middle or the centre of design and plus one and minus one (+1 and -1) as a distances from the zero in both directions. The first order orthogonal system is more efficient as it shows very less variance [15]. From table 2, sum of product input factor columns is zero, hence system is orthogonal. Here for analysis of data, Minitab software is used. The fitted first order Metatamodels can be expressed as,

$$V = 0.8912 - 0.0563x_1 + 0.0487x_2 + 0.2062x_3 \quad (2)$$

$$P = 0.2950 + 0.0850x_1 + 0.0525x_2 + 0.1050x_3 \quad (3)$$

The validity of these models are checked with the help of following statistical tests,

- Normality test
- Regression analysis test
- Analysis of variance test
- Lack of fit test

The regression equation expressing *V* as a function of x_1 , x_2 , x_3 is given by

$$V = 0.891 - 0.0562 x_1 + 0.0487 x_2 + 0.206 x_3 \quad (4)$$

Table 3. Regression analysis

Independent Variables	Coefficients	S.E. Coefficients	Value of T factor	Value of P factor
Constant	0.89125	0.02253	39.55	0.000
x_1	-0.05625	0.02253	-2.50	0.067

x_2	0.04875	0.02253	2.16	0.097
x_3	0.20625	0.02253	9.15	0.001

$$S = 0.0637377, R^2 = 95.9\%, R^2(\text{adj}) = 92.9\%$$

Table 4. Variance Analysis

Source	Deg.Fr	Sum.Sq	Mn. Sq	F Value	P Value
Reg.	3	0.3846	0.1282	31.56	0.003
Res. Er.	4	0.0162	0.0040		
Total	7	0.4008			

The regression equation expressing *P* as a function of x_1 , x_2 , x_3 is given by

$$P = 0.295 + 0.0850 x_1 + 0.0525 x_2 + 0.105 x_3 \quad (5)$$

Table 5. Regression analysis

Independent Variables	Coefficients	S.E. Coefficients	Value of T factor	Value of P factor
Constant	0.29500	0.02678	11.02	0.000
x_1	0.08500	0.02678	3.17	0.034
x_2	0.05250	0.02678	1.96	0.121
x_3	0.10500	0.02678	3.92	0.017

$$S = 0.0757463, R^2 = 88.0\%, R^2(\text{adj}) = 79.0\%$$

Table 6. Variance Analysis

Source	Deg. Fr.	Sum. Sq	Mn. Sq	F Value	P Value
Reg.	3	0.1680	0.0560	9.76	0.026
Res. Er.	4	0.0229	0.0057		
Total	7	0.1910			

Here, the normal probability of *V* and *P* is used to check effectiveness of developed models. From Fig.3 and Fig.4 it is observed that the residual plots of both response variables follows linear relationship hence normality test is said to be satisfied.



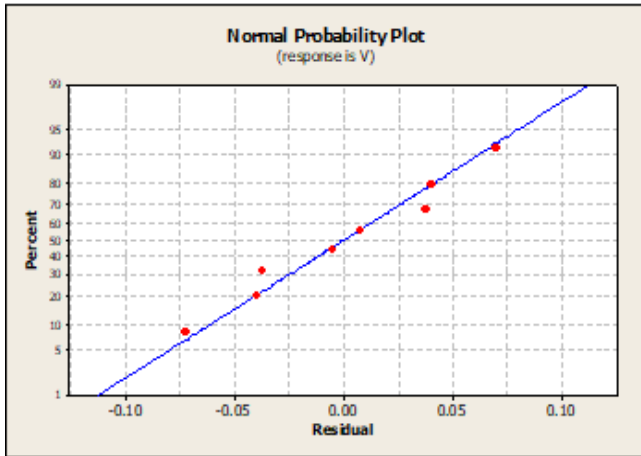


Fig. 3. Normal probability plot for V

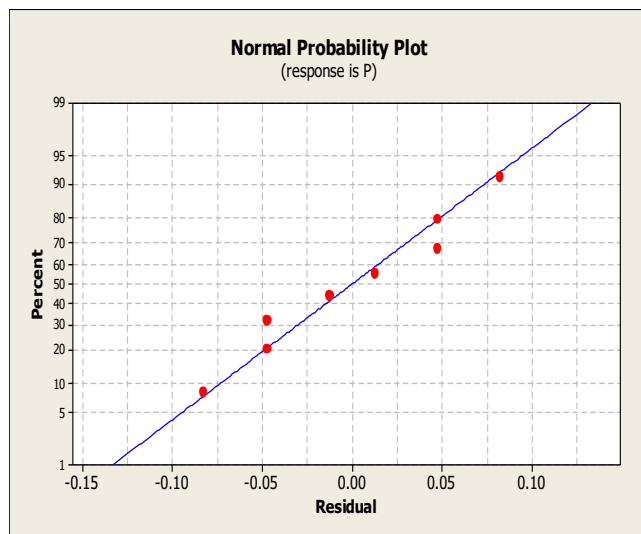


Fig. 4. Normal probability plot for P

The statistical regression analysis test is a hypothesis test which is used to determine relation between dependent variable (response) and independent variables (input factors). Here the hypothesis used is,

$$H_0 : \beta_1 = \beta_2 = \beta_3 = 0 \quad \text{vs} \\ H_1 : \beta_j \neq 0 \quad \text{for minimum one } j$$

From statistical regression analysis test for V, at $\alpha=0.05$ $F_{0.05,3,4}=6.591 < F=31.56$.

From Table 6, $P\text{-value} (0.003) < \alpha (0.05)$.

Also from regression analysis and variance analysis test for P, at $\alpha=0.05$

$F_{0.05,3,4}=6.591 < \text{observed } F=9.76$ and $P\text{-value} (0.026) < \alpha (0.05)$. Therefore, the null hypothesis can be rejected i.e. all variables contributes significantly to particular response variable.

From statistical regression analysis test, the calculated coefficient of determination can be used to

determine how developed model effectively fits the experimental data. When values of coefficient of determination (R^2) nearly approaching 1, it indicate that the developed regression equation fits the sample input data effectively. For both response variables, the calculated coefficient of determination are close to 1, hence the developed regression equations fits input data effectively.

The individual effect on input factors on output factors can be shown using main effect plots. More slop in a plot indicate large effect of that input factor on output factor [16][17]. The figures 5 and 6 shows main effect plots for response variables V and P.

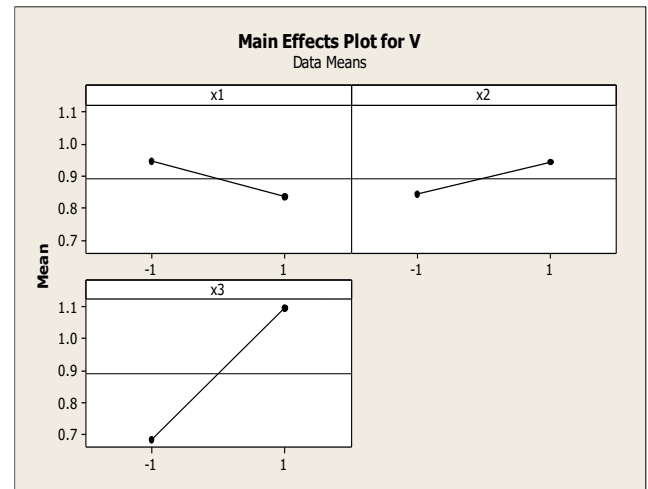


Fig 5. Main effect plot for output voltage

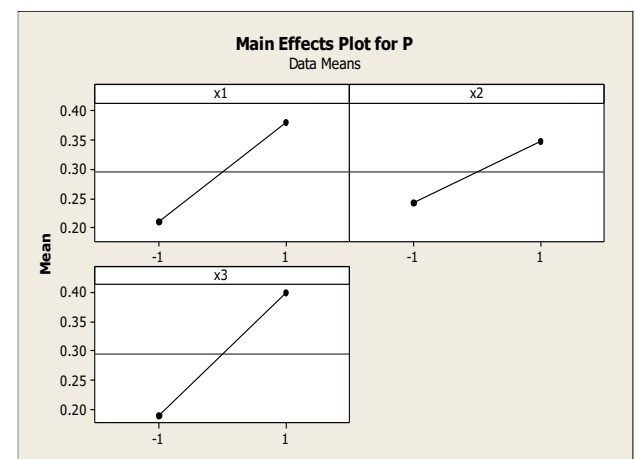


Fig 6. Main effect plot for power density

From Fig. 5 and Fig. 6 it is clear that there is an effect of all input factors on output factors.

To find which independent variable significantly affects the particular dependent variable, a statistical t-test is used. For test statistic following hypothesis is used,

$$H_0: \theta_{x1} = 0 \quad H_1: \theta_{x1} \neq 0$$



$$\begin{array}{ll}
 H_0: \beta_{x2} = 0 & H_1: \beta_{x2} \neq 0 \\
 H_0: \beta_{x3} = 0 & H_1: \beta_{x3} \neq 0
 \end{array}$$

To check hypothesis, the level of significance used is 5 %.
For output variable V ,

$$\begin{array}{l}
 |t_{x1}| = 2.50 > t_{0.05,4} = 1.53 \\
 |t_{x2}| = 2.16 > t_{0.05,4} = 1.53 \\
 |t_{x3}| = 9.15 > t_{0.05,4} = 1.53
 \end{array}$$

As observed $|t_0| > \text{critical value } t_{\alpha, N-q-1}$ hence null hypothesis is rejected.

For output variable P ,

$$\begin{array}{l}
 |t_{x1}| = 3.17 > t_{0.05,4} = 1.53 \\
 |t_{x2}| = 1.96 > t_{0.05,4} = 1.53 \\
 |t_{x3}| = 3.92 > t_{0.05,4} = 1.53
 \end{array}$$

As all t-statistic values are found to be more than t critical values hence null hypothesis is rejected.

First Order Center Point Design Analysis

To check lack of fit for both response variables V and P , here center point design analysis is used. The center point design consists of n_f number of factorial points and $n_c = 3$ center point observations of each response variables [17][18].

To test lack of fit for V , $F_L = MS_{LOF}/MS_{PE} = 0.036$

$F_{\alpha, nd-q-1, N-nd} = 19.296$ and as $F_L < F_{\alpha, nd-q-1, N-nd}$, ($nd = 8+1$),

the evidence for lack of fit at $\alpha = 0.05$ can be rejected.

Similarly for response variable power density, $F_L = MS_{LOF}/MS_{PE} = 0.019$, $F_{\alpha, nd-q-1, N-nd} = 19.296$. As $F_L < F_{\alpha, nd-q-1, N-nd}$, the evidence for lack of fit can be rejected. Therefore the first order model can effectively be used to represent true response surface.

Counter plots for response factors V and P are shown figure 7 and figure 8 respectively. How a particular response variable relates with two input variable at a time that can be judged from counter plots. As there are three input factors, one factor required to be hold at constant level while plotting the other two input factors. Counter plots for response variables V and P are shown in figure 7 and figure 8 respectively.

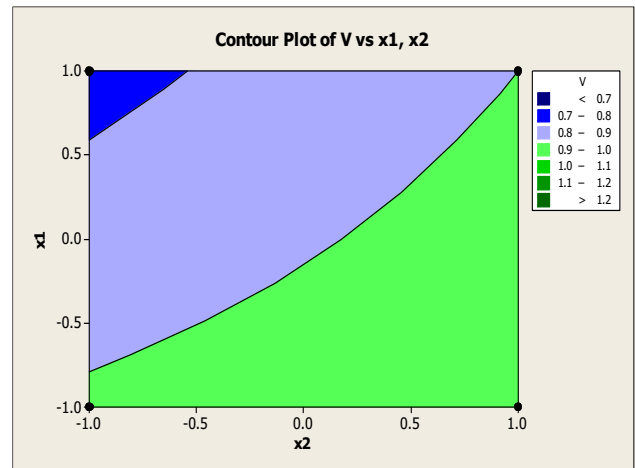


Fig. 7(a). Counter plot for V vs x_1, x_2

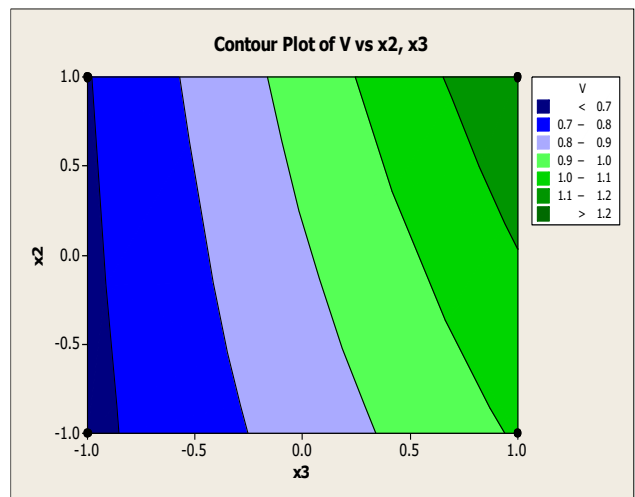


Fig. 7(b). Counter plot for V vs x_2, x_3

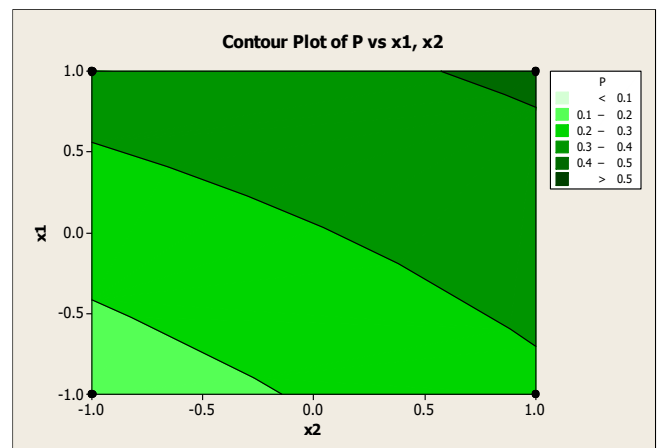
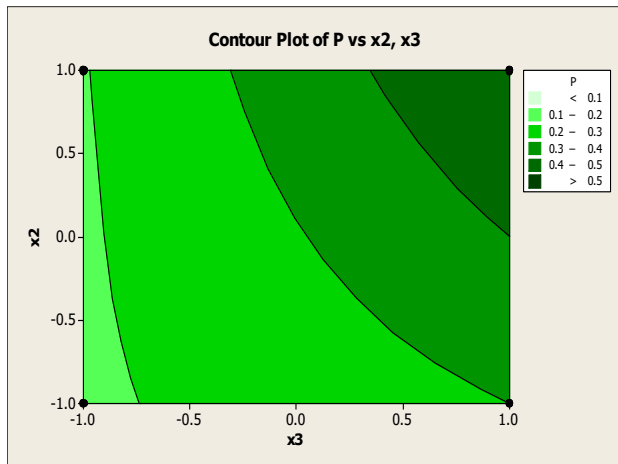


Fig. 8(a). Counter plot for P vs x_1, x_2

Fig. 8(b). Counter plot for P vs x_2, x_3

For flat and tilted response surfaces, the counter lines are always parallel. However, from the counter plot of response variable V vs variables x_1 - x_2 and from the counter plot of response variable P vs variables x_2 - x_3 , the counter lines are not parallel which indicates that there exist curvature in response surface and hence there is a need to analyze higher order model.

Analysis of Higher Order Model Using Response Surface

Curvature in the response surface of first order model indicates that the first order model is insufficient to represent response effectively. To fit second order models, the central composite design (CCD) is proposed here. The CCD consists of one or more axial points, factorial points and center points.

Orthogonal Central Composite Design

The orthogonal CCD needs one observation at each of the n_f factorial points and $2q$ defined axial points and also extra n_c observations at the center. Selecting proper value for significant factor α and n_c , the orthogonal CCD with minimum observations can be achieved [19][20]. Considering $\alpha = 1.215$ and $n_c = 1$, the 15-run CCD matrix is shown in table 7.

Table 7. Central composite design matrix

x_1	x_2	x_3	V	P
-1	-1	-1	0.73	0.10
1	-1	-1	0.62	0.27
-1	1	-1	0.75	0.11
1	1	-1	0.64	0.28
-1	-1	1	1.10	0.18
1	-1	1	0.92	0.42
-1	1	1	1.21	0.45

1	1	1	1.16	0.55
0	0	0	0.97	0.28
1.215	0	0	0.92	0.440
-1.215	0	0	1.05	0.120
0	1.215	0	0.96	0.276
0	-1.215	0	0.4	0.118
0	0	1.215	1.05	0.310
0	0	-1.215	0.64	0.190

This design consists of 15 observations and 6 axial points with 1 centre point.

Response Surface Regression: V versus x_1, x_2, x_3

Table 8. Evaluated Regression Coefficients for V

Predictor	Coeff.	S.E. Coeff.	Value of T factor	Value of P factor
Constant	0.8643	0.0911	9.48	0.000
x_1	-0.0674	0.0508	-1.32	0.242
x_2	0.1187	0.0508	2.33	0.067
x_3	0.2383	0.0508	4.68	0.005
$x_1 * x_1$	0.1552	0.0979	1.58	0.174
$x_2 * x_2$	-0.1497	0.0979	-1.52	0.187
$x_3 * x_3$	0.0152	0.0979	0.15	0.882
$x_1 * x_2$	0.0239	0.0723	0.33	0.754
$x_1 * x_3$	-0.0018	0.0723	-0.02	0.981
$x_2 * x_3$	0.0572	0.0723	0.79	0.465

$S = 0.138586$ PRESS = 0.799359
 $R^2 = 87.42\%$ $R^2(\text{pred}) = 0.00\%$ $R^2(\text{adj}) = 64.78\%$

$$V = 0.864 - 0.0674x_1 + 0.12x_2 + 0.24x_3 + 0.16x_1^2 - 0.15x_2^2 + 0.0152x_3^2 + 0.024x_1x_2 + 0.057x_2x_3 \quad (6)$$

Table 9. Variance Analysis for V

Term	Deg. Fr.	Sm.S	Ad. Sm. S.	Ad.Mn. S	Value of F factor	Value of P factor
Reg.	9	0.6673	0.6673	0.0741	3.86	0.075
Linr.	3	0.5596	0.5596	0.1865	9.71	0.016
x_1	1	0.0337	0.0337	0.0337	1.76	0.242
x_2	1	0.1046	0.1046	0.1046	5.45	0.067
x_3	1	0.4213	0.4213	0.4213	21.9	0.005
Sq.	3	0.0935	0.0935	0.0311	1.62	0.296
$x_1 * x_1$	1	0.0481	0.0481	0.0482	2.51	0.174
$x_2 * x_2$	1	0.0448	0.0448	0.0448	2.34	0.187
$x_3 * x_3$	1	0.0004	0.0004	0.0004	0.02	0.882
Interaction	3	0.0141	0.0141	0.0047	0.25	0.862
$x_1 * x_2$	1	0.0021	0.0021	0.0000	0.11	0.754
$x_1 * x_3$	1	0.0000	0.0000	0.0000	0.00	0.981



$x_2 * x_3$	1	0.0120	0.0120	0.0120	0.63	0.465
Residual Error	5	0.0960	0.0960	0.0960		

Response Surface Regression: P versus x_1, x_2, x_3

Table 10. Estimated Regression Coefficients for P

Term	Coeff.	S.E. Coeff.	Value of T factor	Value of P factor
Constant	0.2297	0.0401	5.721	0.002
x_1	0.1185	0.0224	5.292	0.003
x_2	0.0678	0.0224	3.030	0.029
x_3	0.1093	0.0224	4.881	0.005
$x_1 * x_1$	0.0668	0.0431	1.549	0.182
$x_2 * x_2$	-0.0162	0.0431	-0.376	0.723
$x_3 * x_3$	0.0368	0.0431	0.853	0.433
$x_1 * x_2$	-0.0258	0.0318	-0.811	0.454
$x_1 * x_3$	-0.000	0.0318	-0.000	1.000
$x_2 * x_3$	0.0701	0.0318	2.202	0.079

$S = 0.0610251$ PRESS = 0.171368

$R^2 = 93.31\%$ $R^2(\text{pred}) = 38.47\%$ $R^2(\text{adj}) = 81.28\%$

$$P = 0.23 + 0.12x_1 + 0.068x_2 + 0.11x_3 + 0.067x_1^2 - 0.016x_2^2 + 0.037x_3^2 - 0.026x_1x_2 - 0.07x_2x_3 \quad (7)$$

Table 11. Variance Analysis for P

Terms	Deg. Fr	Seq Sm. Sq	Adj Sm. Sq	Adj Mn. Sq	Value of F factor	Value of P factor
Reg.	9	0.2598	0.2598	0.0288	7.75	0.018
Linr.	3	0.2272	0.2272	0.0757	20.34	0.003
x_1	1	0.1042	0.1042	0.1042	28.01	0.003
x_2	1	0.0341	0.0341	0.0341	9.18	0.029
x_3	1	0.0887	0.0887	0.0887	23.83	0.005
Sq.	3	0.0121	0.0121	0.0040	1.09	0.434
$x_1 * x_1$	1	0.0089	0.0089	0.0089	2.40	0.182
$x_2 * x_2$	1	0.0005	0.0005	0.0005	0.14	0.723
$x_3 * x_3$	1	0.0027	0.0027	0.0027	0.73	0.433
Inter.	3	0.0205	0.0205	0.0068	1.83	0.258
$x_1 * x_2$	1	0.0024	0.0024	0.0024	0.66	0.454
$x_1 * x_3$	1	0.0000	0.0000	0.0000	0.00	1.000
$x_2 * x_3$	1	0.0180	0.0180	0.0180	4.85	0.079
Res. Er.	5	0.0186	0.0186	0.0037		
Total	14	0.2785				

From regression analysis and variance analysis tests, the

final second order Metamodels can be expressed as

$$V = 0.864 - 0.0674x_1 + 0.12x_2 + 0.24x_3 + 0.16x_1^2 - 0.15x_2^2 + 0.0152x_3^2 + 0.024x_1x_2 + 0.057x_2x_3$$

$$P = 0.23 + 0.12x_1 + 0.068x_2 + 0.11x_3 + 0.067x_1^2 - 0.016x_2^2 + 0.037x_3^2 - 0.026x_1x_2 - 0.07x_2x_3 \quad (8)$$

Counter plots are very useful to find shape of response surface and locating optimum response approximately. Fig. 9 and Fig.10 represent counter plots and response surfaces for response variable V whereas Fig. 11 and Fig.12 represent counter plots and response surfaces for response variable P . From the plot it is clear that there is a curvature and this curvature in the response plots clearly indicate the model consists of quadratic terms.

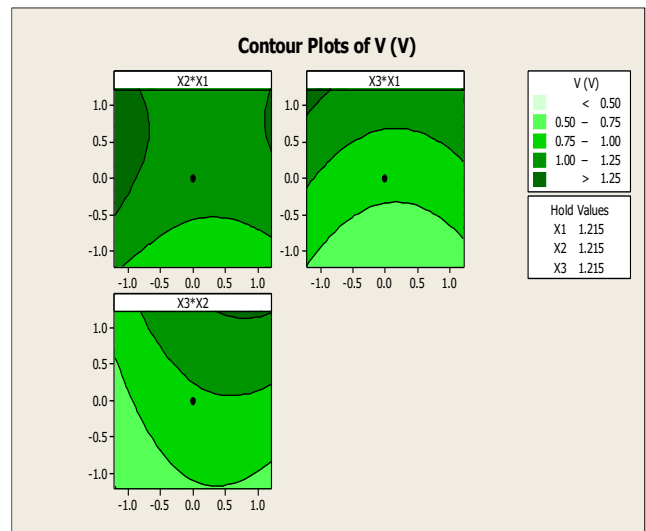


Fig. 9. Counter plots for V

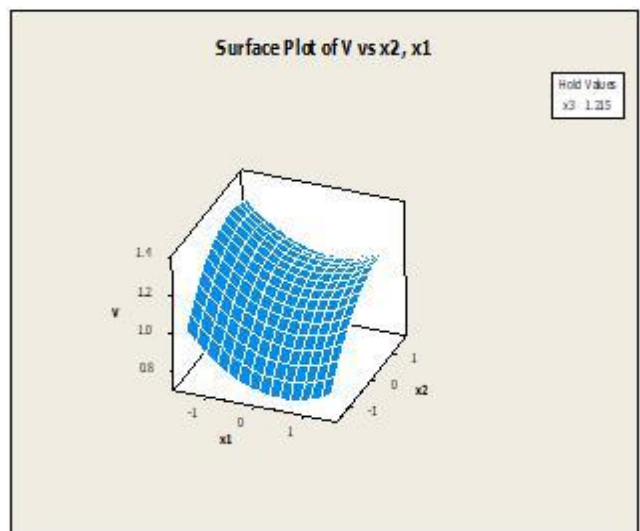


Fig. 10(a). Response surface plot for V vs x_1, x_2 .



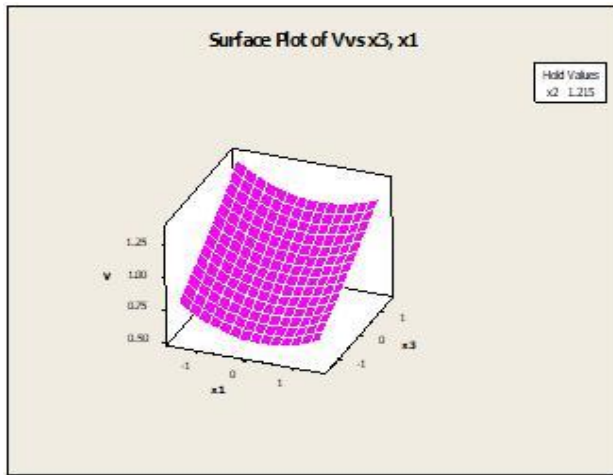


Fig. 10(b). Response surface plot for V vs x_1, x_3 .

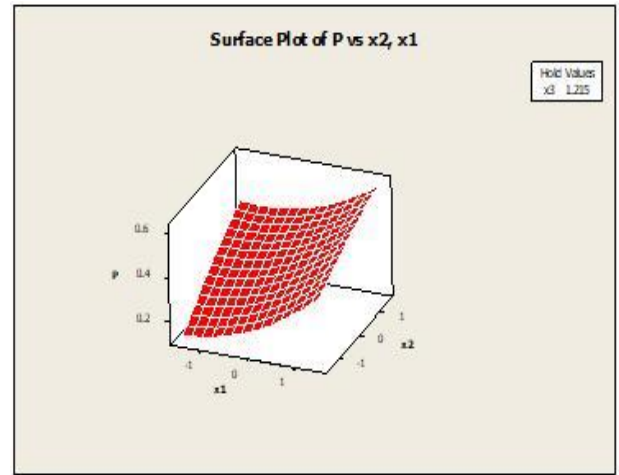


Fig. 12(a). Response surface plot for P vs x_1, x_2 .

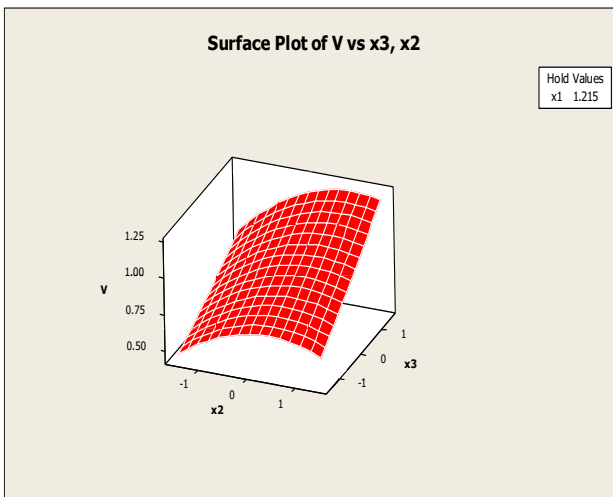


Fig. 10(c). Response surface plot for V vs x_3, x_2 .

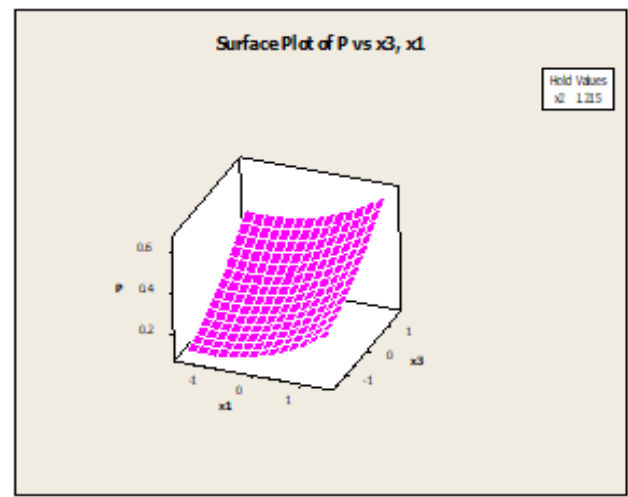


Fig. 12(b). Response surface plot for P vs x_1, x_3 .

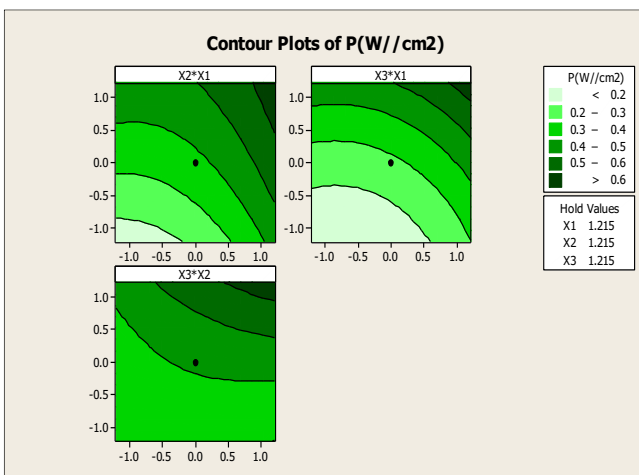


Fig.11. Counter plots for P

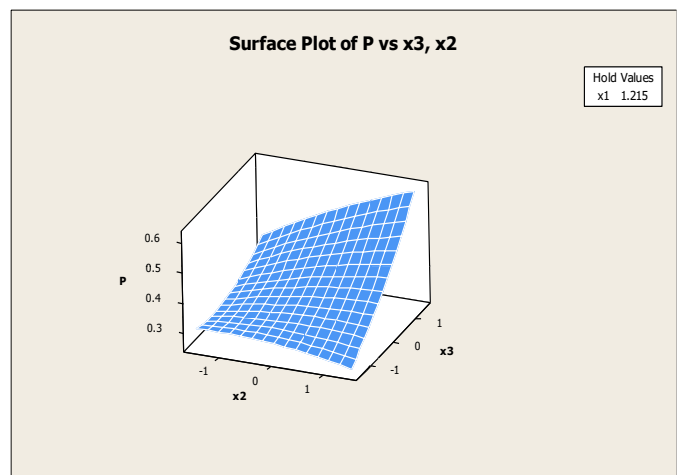


Fig. 12(c). Response surface plot for P vs x_3, x_2 .

Optimization of Metamodels

The developed second order model explains

quadratic surfaces which includes maximum, minimum, saddle and ridge. Existence of optimum in quadratic surface is the indication of presence of a stationary point. The combine existence of input variables at which the quadratic surface is either max or min in all directions is called as stationary point. If the stationary point is max in some direction and min in another direction, then the stationary point is considered to be saddle point. To find the stationary point, consider the fitted second order model for fuel cell voltage

$$\hat{y}_v = \hat{\beta}_0 + x'b + x'Bx \quad (9)$$

$$\frac{d\hat{y}_v}{dx} = b + 2Bx = 0 \quad (10)$$

$$x_s = -\frac{1}{2} B^{-1} b \quad (11)$$

where,

'b' represents single column matrix of regression coefficients and 'B' represents a symmetric matrix of quadratic coefficients and half the mutual quadratic coefficients. The response factors at the stationary point can be calculated from

$$\hat{y}_s = \hat{\beta}_0 + \frac{1}{2} x'_s b \quad (12)$$

For response variables, V and P, the stationary points are calculated as

$$x_s = \begin{bmatrix} 0.2343 \\ -0.7953 \\ -0.6389 \end{bmatrix} \quad \text{For V, and}$$

$$x_s = \begin{bmatrix} -0.9123 \\ -0.1251 \\ -1.3682 \end{bmatrix} \quad \text{For P}$$

Using equation,

$$\hat{y}_s = \hat{\beta}_0 + \frac{1}{2} x'_s b \quad (13)$$

The values of the response variables, fuel cell output voltage and power density corresponding to calculated stationary points are given by,

$$V = 0.732 \text{ V}$$

$$P = 100 \text{ mW/cm}^2$$

Conclusion

Statistical design of experiment, response surface methodology is an effect tool to develop Metamodels for any dynamic system to analyze effect of one or more input

factors on one or more output factors. The first and second order Metamodels developed for both response factors of PEM fuel cell are accurate and validated using various statistical tests. The calculated stationary points specify operation region of the PEM fuel cell for optimum response. The presented method can be used for modeling, optimization and feasibility study of other fuel cells and fuel cell systems.

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