CHAPTER 4

OPTIMIZATION OF PROCESS PARAMETERS BY RSM

The optimization of any system or process is defined as enhancing the performance of the system or process so that maximum benefit can be obtained. The current effort focuses on the optimization of operating parameters using box behnken design (BBD) to obtain maximum power density from the hydrogen-based PEMFC with the help of statistical method response surface methodology (RSM). There are numerous factors, including pressure, stoichiometry, humidity, cell operation temperature, reactant gas temperature, and component shape, which control the fuel cell system performance. According to the information provided, the most crucial environmental aspect that prompted this search is the reduction of emissions using hydrogen at anode side as fuel. It is often regarded as a renewable fuel capable of eliminating dependency on fossil fuels. The hydrogen fuel would be renewable when it is produced from water electrolysis or photocatalytic splitting from water using renewable energy i.e., sunlight (Saleem et al., 2024). The first step in studying hydrogen-based fuel cell is to improve the materials employed in terms of cost and performance, to address issues that arose during application, during the design phase, and to enhance the operating conditions of the fuel cell. These have been carried out using a variety of experimental and numerical methods. First among these investigations are design of experiments (DOE) and response surface methodology (RSM). Due to the limited number of tests, these mathematical techniques have been used in engineering science and technology almost last 10 years. Fuel cell applications have been widespread for the previous 15 years and continue to be so today and further also. Yu et al., (2008) used fractional factorial DOE design with an orthogonal array of the Taguchi Method to determine the best operating parameters for a PEMFC. Meiler et al., (2009) employed a DOE method also known as D-optimal design to lower the expense of the experimental design. Pressure and relative humidity were chosen as operating parameters for PEM fuel cells in their study. The D-optimal design strategy reduced the number of experimental measurements from 405 to 50 utilizing only four input parameters. The cost of engineering design was decreased, and fuel cell performance was enhanced, as a result of this strategy. The article by Kravos et al. (2021) presented the influence of various operational settings utilizing D-optimal design. Moreover, their findings show that, in contrast to hydrogen and oxygen flow rates, pressure has little or no impact on cell performance. The major aim of the current study is to assess how well a PEM fuel cell performs while the hydrogen content and other effective parameters are kept at optimum condition. To do this, a series of effective operating variables was varied to find the highest power.

A mathematical and statistical method known as the RSM correlates the results or response from the cell with the input process variables. It helps to create the model, evaluate the effects of the input process parameters, and establish the ideal circumstances for the desired results (Huang et al., 2018; Myers et. al., 2016; Wu and Gu 2010). Based on experimental data, the RSM helps in the development of a polynomial equation to predict the best response as a function of the effective input variables (Okur et al., 2013; San et al., 2014). According to Allaedini et al., (2016), the effects of parameters on the response examined using RSM reveal interactive effects among variables and illustrate the overall effects on the process. The RSM-based optimization studies can be broken down into three parts. Finding the independent parameters and levels of experiments is the initial stage. The model equation is predicted and verified in the second stage, which also involves choosing an experimental strategy. The final phase involves determining the process output as a function of the independent variables and ideal circumstances (Bas and Boyaci 2007).

The preliminary experiments are used to determine the experimental domain, which is the upper and lower limits of the experimental parameters. To determine the factors that have the greatest impact on the performance of PEMFC, parameters must be screened. The preliminary experiments also yielded the most influential and effective parameters. As per literature, the cathode electrocatalyst loading (A), cell operating temperature (B) and hydrogen flow rate (C) are considered as influencing factors in the current experiment for improving the cell performance in PEMFC. As already mentioned, among all the synthesized cathode electrocatalyst Pt-Ni(3:1)/C_{AB}-EG showed the greatest performance in terms of power density in PEMFC. Thus, in the current investigation, Pt-Ni(3:1)/C_{AB}-EG was used to optimize the effective process parameters. For the optimization investigation, commercial Pt/C_{HSA} was employed as the anode electrocatalyst. The purpose of the present study is to determine the optimum values of independent variables that will allow hydrogen-based PEMFC to perform at its highest power density. The cathode electrocatalyst loading, cell operating temperature and hydrogen flow rate are the independent variables. Utilizing analysis of variance (ANOVA) and experimental data that can be reliably predicted by the model, the generated model was validated. The levels and limits of the independent variables are shown in the Table 4.1.

Table 4.1 Levels and limits of independent variables studies in the BBD

Independent Variables	**Low level (−1)**	**Middle level (0)**	**High level (+1)**
A – Cathode loading	0.75	1	1.25
B – Cell temperature	50	60	70
C – Hydrogen flow rate	40	50	60

The number of experiments required to perform BBD are determined using Equation (4.1) (Choudhary and Pramanik 2021).

$$N = 2k(k - 1) + cp \tag{4.1}$$

All 17 experiments were carried out to obtain the experimental response in terms of power density. A quadratic model was chosen (Choudhary and Pramanik 2021; Panjiara and Pramanik 2020; Myers et al., 2016) as it was found to be one of the best fitted models with a significant response. The ANOVA analysis was carried out to determine the number of central points and the number of factors used in the experiments (Equation 4.2). Where Y is the response i.e., maximum power density and x_i and x_j are the independent factors. β_0, β_i, β_{ii}, and β_{ij} represents the linear parameter, i represents the quadratic parameter, and ij represents the interaction parameter.

$$Y = \beta_o + \sum_{i=1}^{k} \beta_i \times X_i + \sum_{i=1}^{k} \beta_{ii} \times X_i^2 + \sum_{i \text{ and } j=1,\, i \neq j}^{k} \beta_{ij} \times X_i \times X_j \tag{4.2}$$

The developed model equation predicts the optimized process parameters and RSM results are presented in the chapter 5, section 5.2.4 in (Page no.113).