International Journal of Advanced Technology in Engineering and Science
Vol. No.9, Issue No. 05, May 2021
www.ijates.com
ijates
ISSN 2348 - 7550

Prediction modelling and optimization of compact methanol steam reformer using Gaussian process regression (GPR) and Response surface optimization.

Sibun Raj Rout1, Dr. Prashant Nehe2

1(PG Student Mechanical Engineering Department Gokhale Education Society's R. H. Sapat College of Engineering, Management Studies and Research, Savitribai Phule Pune University Nasik, Maharashtra, Indi)

2(Associate Professor, Mechanical Engineering Department, Gokhale Education Society's R. H. Sapat College of Engineering, Management Studies and Research. Savitribai Phule PuneUniversity Nasik, Maharashtra, India)

ABSTRACT:

This paper propose a new predictive model based on Gaussian process regression (GPR) algorithm with matern 5/2 and matern 3/2 kernel for estimating the yield of a methanol steam reformer. The input parameters consist of reforming temperature and feed rate while the target output includes methanol conversion, hydrogen production and carbon-monoxide generation. The high value of coefficient of determination (R^2=1) acquired indicates that the predicted rate of target output is strongly correlated with the observed value. The Least root mean square (RMSE) for methanol conversion and hydrogen generation is obtainedbymatern 3/2 kernel and carbon-monoxide generation by matern 5/2kernel. Response surface optimization (RSO) optimizes the input parameter by maximizing the methanol conversion and minimizing the carbon-monoxide. The inlet feed flow rate of 29.3939cm^3/hr. and reformer temperature of 239.798˚C is been observed with the application of multiobjective optimization.

Keywords:*Response surface optimization (RSO), Gaussian process regression (GPR), methanol steam reformer, matern 3/2 kernel and matern 5/2 kernel*

1. INTRODUCTION

The improvement within the performance of the many portable electronic devices in terms of miniaturization has become significant during the last decade. Therefore, nowadays researchers are focusing on the event of portable power sources capable of delivering power in 0.1–100Wrange for potential usage in combat situations also as small electronic devices. Recent growth toward the event of fuel cells proposes an alternate power source thanks to their high-energy efficiency and eco-friendly nature. [1]Fuel cells need endless supply of hydrogen gas for his or her operation and hydrogen is named as a fuel of future. Hydrogen based proton exchange membrane fuel cells (PEMFCs) have the potential of providing energy storage densities several times above those achievable using current state-of-the-art lithium-ion batteries. [2]Hydrogen (H_2) has become one among the foremost interesting clean energy carriers for the near future due to the depletion of non-renewable fossil fuels, the expansion in heating, and therefore the rise in serious pollution problems. H_2 are often produced from sustainable liquid fuels or alcohols like methanol. Methanol, which is quickly available and may be produced from renewable sources, is taken into account as the optimal potential H_2 source for 2 main reasons. Firstly, methanol is often catalytically converted to a H_2-rich stream at a comparatively coldness range (200 °C to 400 °C) with no requirement for desulfurization or pre-reforming processes. Secondly, there's no C–C bond within the methanol structure (unlike within the easier to supply ethanol), which minimizes the danger of coke formation. There are four main reactions to supply H_2 from methanol, being the decomposition (DM), steam reforming (SRM), partial oxidation (POM) and auto thermal reforming (ARM) of methanol. Comparing the stoichiometric H_2 production among these reactions, the SRM method yields more H_2 with no carbon monoxide gas (CO) content, as shown in Eq. [1,2,3]. [3]

Steam Reforming:

$CH_3OH_{(g)} + H_2O_{(g)} \leftrightarrow 3H_{2\,(g)} + CO_{2\,(g)}$ $\Delta H = +49.5$ KJ/mol…………….... (1)

Decomposition:

$CH_3OH_{(g)} \leftrightarrow 2H_{2(g)} + CO_{(g)}$ $\Delta H = +49.5$ KJ/mol…………….... (2)

Water-gas shift:

$CO_{(g)} + H_2O_{(g)} \leftrightarrow H_{2\,(g)} + CO_{2\,(g)}$ $\Delta H = +49.5$ KJ/mol…………….... (3)

Researcher has however begun to investigate the utilization of machine learning algorithms in methane steam reforming. Bamidele Victor Ayodeleet al [4] utilised artificial neural network to model the hydrogen production rate from methane dry reforming with the utilisation of the presence of Co/Pr_2O_3as the catalyst. The study investigates the speed of CO and H_2 production and observed good result in all cases ($R^2 > 0.999$). Computational intelligence are slow in generating results due to theiterative tuning of the models user-defined parameters and the steepest-gradient training algorithmsutilized. To beat these issues, a non-parametric approach to regression known as Gaussian processregression (GPR) avoids over fitting by defining a function distribution and setting a previous distributionof unlimited possibilities over the function directly. GPR is additionally known to generalize wellthanks to its preference to a smooth function that accurately explains the training data without manualparameter tuning as has been the case of ANN. After applying GPR the info is employed for performingmulti objective optimize to maximize Methanol Conversation, minimization of Carbon Monoxide for the Methanol Steam Reformer by using Response Surface Optimization.

2. MODELLING METHODOLOGY

2.1 Gaussian processregression (GPR)

A Gaussian process (GP) is an infinite group of random variables of which any of the finite subsets features a continuing joint Gaussian distribution. A GP is represented by a mean function and a covariance function. Since the GP could also be a linear combination of random variables is having a standard distribution, by simplicity, the mean function is usually assumed to be zero. Assuming a training set y of n number of parameters and having an input matrix $X \in R^n$ and output variable $Y \in R$, which is expressed to be a methanol conversion or hydrogen generation. The Gaussian process is therefore represented in Equation (1) as:

$$Y \sim GP\,(m(x),\, k\,(x, x')) \qquad (1)$$

Where GP is Gaussian process, m(x) is that the mean function and k (x, x′) is that the covariance function. The m(x) within the GP represents the arithmetic mean of the function y at the input matrix point x as expressed in Equation (2):

$$m\,(x) = E\,[f(x)] \qquad (2)$$

The k (x, x′) is the confidence level for m(x) as represented in Equation (3). TheCovariance function takes any two arguments such it generates a non-negative covariance matrix K.

$$K\,(x, x') = E\,[(f(x) - m(x))\,(f\,(x') - m\,(x'))] \qquad (3)$$

There are various covariance functions (kernel functions) that can be employed in a GPR as denoted in Equations:

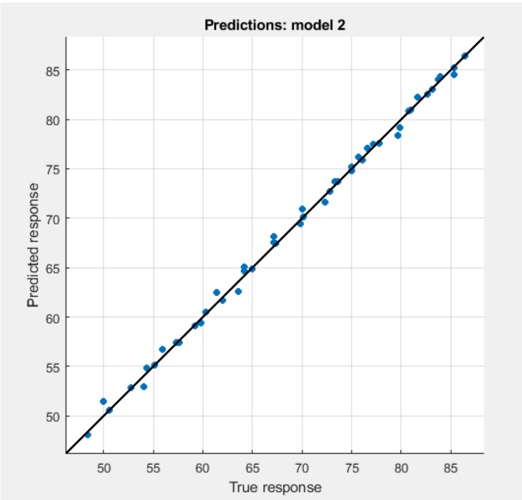
(1) Matern 3/2:

$$K\,(x, x') = \sigma^2_f\,(1 + \sqrt{3r}\,)\,\exp\,[-\sqrt{3r}\,] \qquad (6)$$

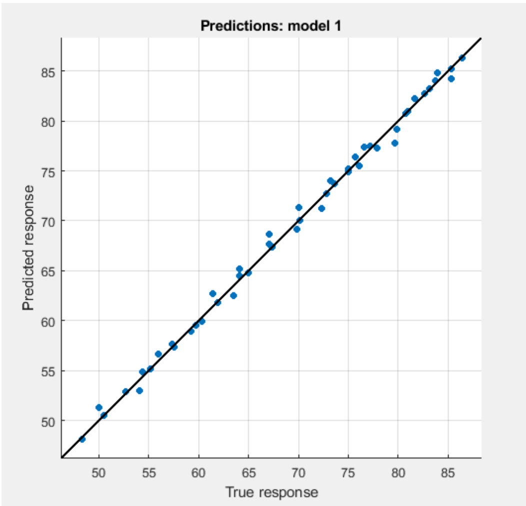
(2) Matern 5/2:

$$K\,(x, x') = \sigma^2_f\,(1 + \sqrt{5r} + \frac{5r}{3})\,\exp\,[-\sqrt{5r}\,] \qquad (7)$$

The predicted Vs Actual response plot is employed to see model performance after training a model. Use this plot to know how well the regression model makes predictions for various response values. The anticipated response of our model is plotted against the particular, true response. An ideal regression model features a predicted response adequate to truth response, so all the points lay on a diagonal line. The vertical distance from the road to any point is that the error of the prediction for that time. A True model has small errors, then the predictions are scattered near the road. Usually an honest model has points scattered roughly symmetrically round the diagonal line. If we will see any clear patterns within the plot, it's likely that we will improve the model. The predicted Vs Actual response plot of matern 5/2 GPR, matern 3/2 for methanol conversion, hydrogen generation, and carbon monoxide gas formation respectively are shown in figure 1, 2, 3.



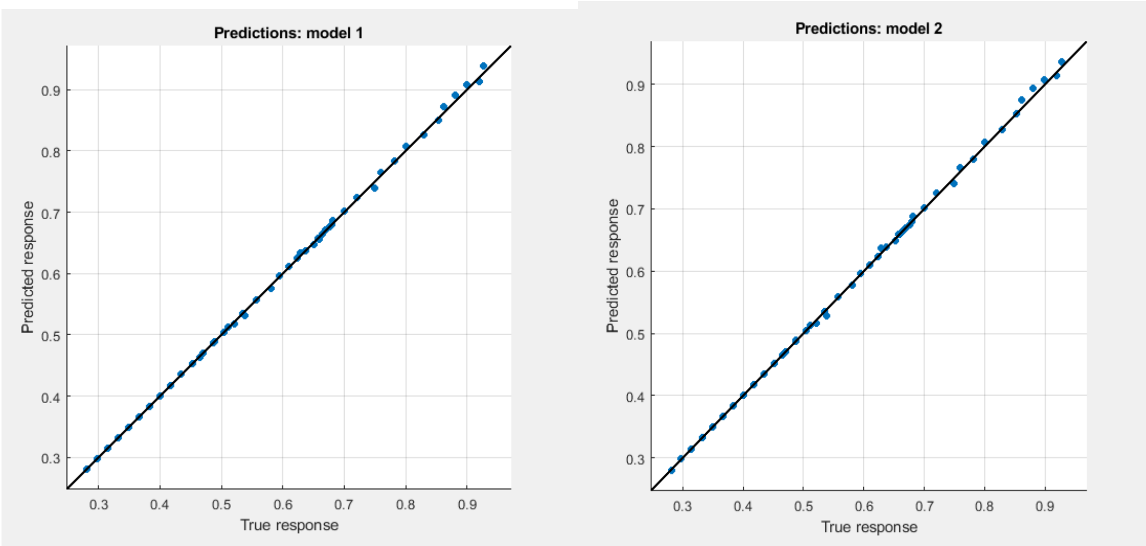
(a) matern 5/2 kernel



(b) matern 3/2 kernel

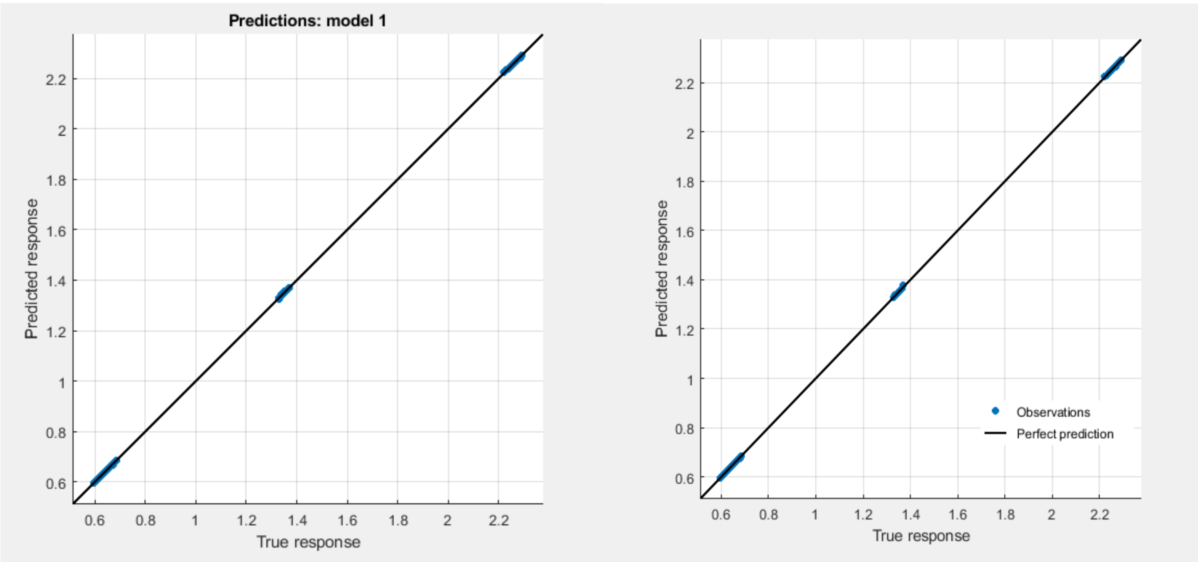
International Journal of Advanced Technology in Engineering and Science
Vol. No.9, Issue No. 05, May 2021
www.ijates.com
ijates
ISSN 2348 - 7550

Fig 1. Predicted vs. Actual plot for methanol conversion by Gaussian Progression Regression



(a) matern 5/2 kernel **(b) matern 3/2 kernel**

Fig 2. Predicted vs. Actual plot for hydrogen generation by Gaussian Progression Regression



(a) matern 5/2 kernel **(b) matern 3/2 kernel**

Fig 3. Predicted vs. Actual plot for carbon monoxide formation by Gaussian Progression Regression

The concept of Gaussian processes is understood as after Carl Friedrich Gauss because it'ssupported the notion of the traditional Gaussian distribution to be an infinite-dimensional generalization of multivariate normal distributions. Every linear combination is evenly distributed; Gaussian process is used in statistical modeling, regression to multiple target values and analyzing mapping in higher dimensions. For each GPR model we'll be (1) Training a knowledge set with GPR models such as Matern 5/2 GPR and Matern 3/2 GPR (2) Plotting the behavior of each algorithm deciding the RMSE, R-Squared Value, MSE, Prediction Speed, Training Time, and (3) Analyzing the results of each Gaussian process regression to determine the similarities and differences of the data. The aim of these trials is to determine if we'll find some interesting behaviors, so we'll find different method to optimize GPR models. Shown below are the varied behaviors of each GPR. Furthermore, the anticipated data is that the used for response surface optimization (RSO) for optimizing input parameters which are input feed flow rate and reforming temperature.

2.2 Response Surface Optimization

The Response Surface Methodology for Design of Experiments (DOE) is employed to hold out Response Surface Optimization. The Reforming Temperature and Inlet Feed flow is taken into account as input response predictors to maximise Hydrogen Formation and Methanol Conversion and carbon monoxide gas is minimized. The following phase is to analyses and interpret the results so valid and sound conclusions are often derived. The Pareto Plot is to be used for the analysis of experimental results. The Pareto plot allows one to detect the factor and interaction effects that are most significant to the processor design optimization study one should house. It displays absolutely the values of the results and draws a reference line on the chart. A Pareto plot is made for the Dataset is shown in Figure 4, 5, 6. Minitab displays absolutely the value of the standardized effects of things when there's a blunder term. There's a main effect when different levels of an element affect the response differently. A main effects plot graphs (figure 7, 8, 9) the response mean for every factor level connected by a line.

2.2.1 Pareto Plot of Factor Effects

The Pareto plot allows one to detect the factor and interaction effects that are most significant to the processor design optimization study one needs to accommodate. It displays absolutely the values of the results and draws a reference line on the chart. The values crosses the reference line are equally important. For instance, for the methanol steam reformer, a Pareto plot is made in Figure 4, 5, 6.

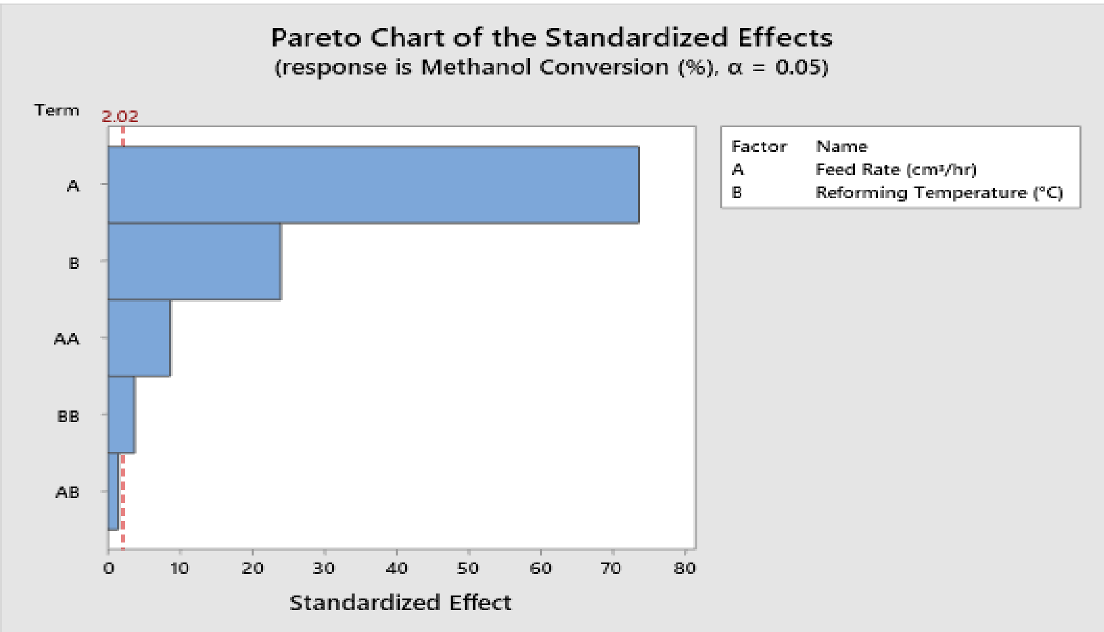


Figure 4: Pareto Effect Methanol Conversion

International Journal of Advanced Technology in Engineering and Science
Vol. No.9, Issue No. 05, May 2021
www.ijates.com
ijates
ISSN 2348 - 7550

From Figure 4 it can be observed that the most impacting factor for methanol conversion are feed rate and reforming temperature as both the factors crosses the reference line as shown in figure 1, Thus both the input factors play a vital role in methanol conversion.

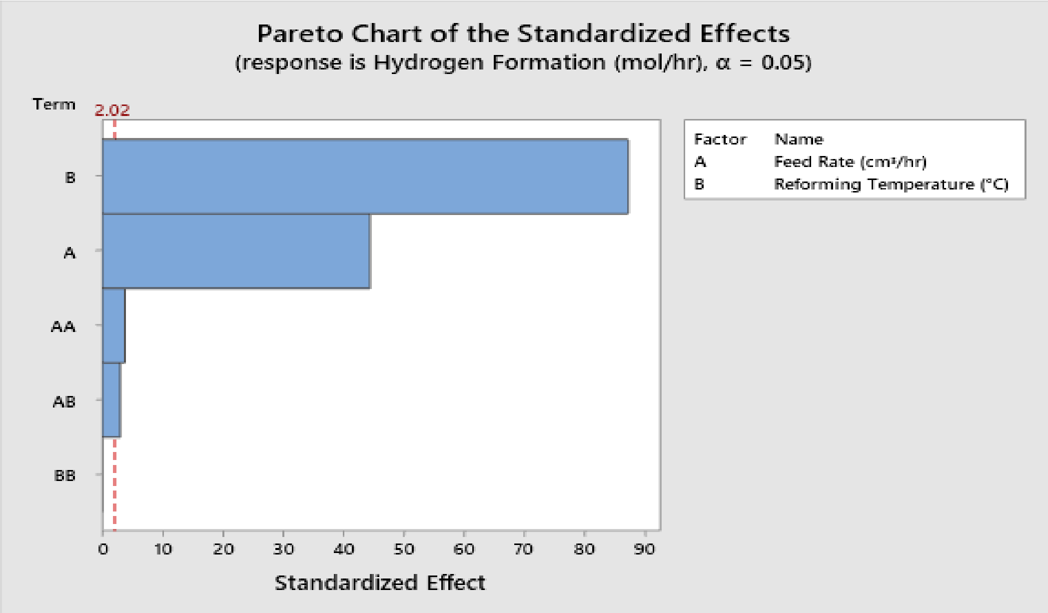


Figure 5: Pareto Effect of Hydrogen Formation

From Figure 5 it can be observed that the most impacting factor for Hydrogen generation are feed rate and reforming temperature as both the factors crosses the reference line as shown in Figure 5, so both the input factors play a vital role in Hydrogen generation .

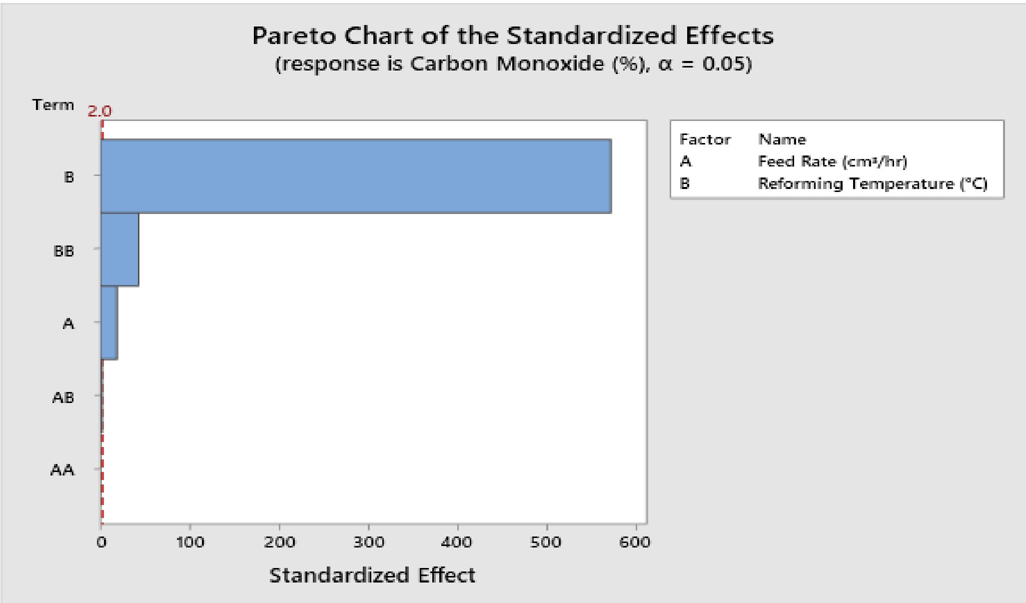


Figure 6: Pareto Effect Carbon Monoxide

From Figure 6 it can be observed that the most impacting factor for Carbon Monoxide is Reforming temperature as compared to the Feed rate.

International Journal of Advanced Technology in Engineering and Science
Vol. No.9, Issue No. 05, May 2021
www.ijates.com
ijates
ISSN 2348 - 7550

2.2.2 Main Effect Plot

The Main Effects plot could be a plot of the mean reaction esteems at each degree of a plan boundary or procedure variable main. One can use this plot to match the relative strength of the results of varied factors. The sign and magnitude of the most impact would tell us the following:

- The sign of the most impact tells us of the direction of the effect, that is, whether the common response value increases or decreases.
- The strength of the effect depends on magnitude.

If the effect of a design or process parameter is positive, it implies that the typical response is higher at a high level instead of a coffee level of the parameter setting. In contrast, if the effect is negative, it implies that the common response at the low-level setting of the parameter is quite at the high level.

The effect of a processor design parameter (or factor) are often mathematically calculated using the subsequent simple equation

$$\mathbf{E_f} = \bar{\mathbf{f}}_{(+1)} + \bar{\mathbf{f}}_{(-1)} \qquad \textbf{(8)}$$

Where $\bar{F}\,(+1)$ = average response at the high-level setting of a factor, and $\bar{F}\,(-1)$ = average response at the low-level setting of a factor.

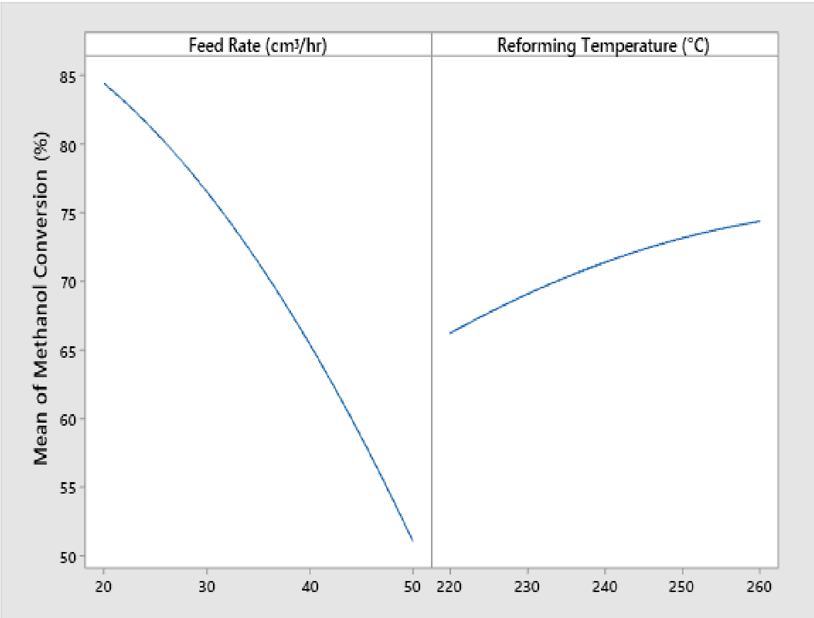


Figure 7: Main Effect Plot Methanol Conversion

From Figure 7, it is observed that methanol conversion decreases with increase in feed rate, but as the reforming temperature increases the methanol conversion also increases, it can also be inferred that for generating high methanol conversion it needs high reforming temperature and less feed rate.

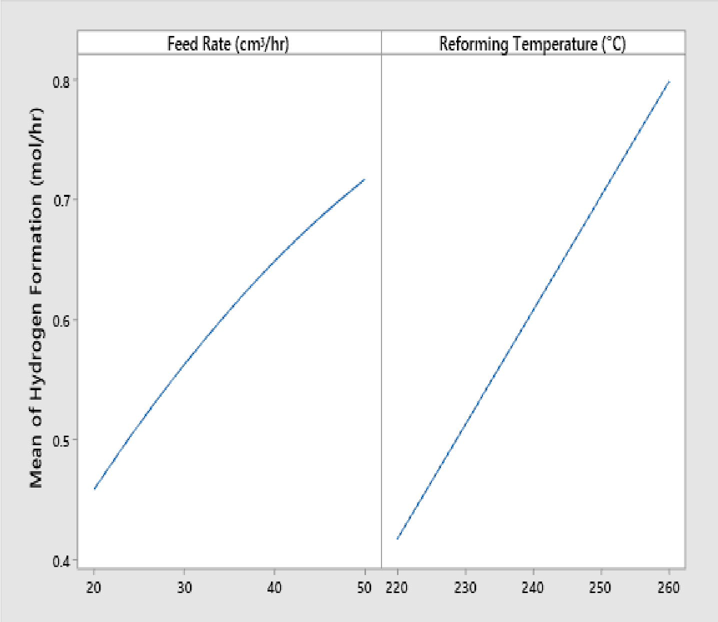


Figure 8: Main Effect Plot Hydrogen Formation

From Figure 8, it is observed that with increasing feed rate and reforming temperature hydrogen generation also increases. To obtain maximum hydrogen generation both feed flow rate and reforming temperature should be maximum.

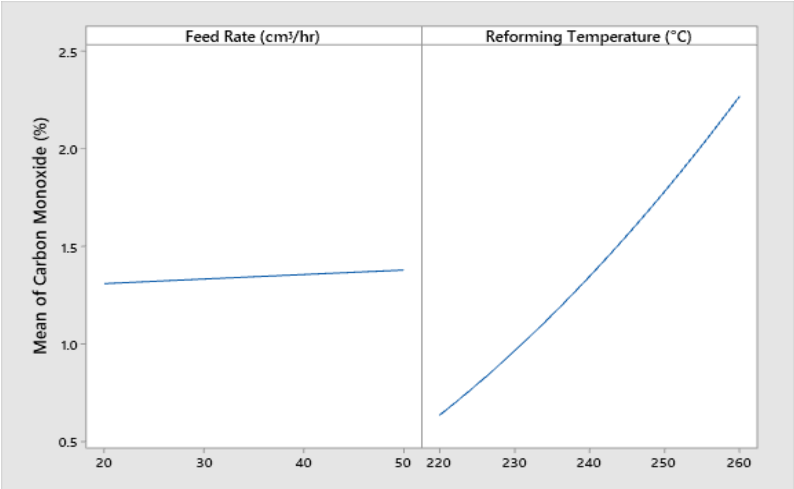


Figure 9: Main Effect Plot Carbon Monoxide Generation

From Figure 9, it is observed that feed flow rate has low effect and Reforming temperature has high effect on carbon monoxide generation. Thus in order to get minimum carbon monoxide reforming temperature needs to be optimized as it plays a major impacting role in increasing carbon oxide therefore it needs to be optimized.

3. Results and discussion

3.1 Gaussian Progression Regression

International Journal of Advanced Technology in Engineering and Science
Vol. No.9, Issue No. 05, May 2021
www.ijates.com
ijates
ISSN 2348 - 7550

Table: Result table for Gaussian Progression Regression for matern 5/2 and matern 3/2 kernel

Factors	Methanol Conversion		Hydrogen Formation		Carbon Monoxide Generation	
	Matern 5/2	Matern 3/2	Matern 5/2	Matern 3/2	Matern 5/2	Matern 3/2
RSME	0.6877	0.54889	0.0038477	0.0035743	0.0010406	0.0013772
R-Squared	1	1	1	1	1	1
MSE	0.47293	0.30128	0.000014805	0.000012776	1.0828E-06	1.8966E-06
MAE	0.51624	0.41281	0.0025498	0.0022276	0.00075245	0.00073563
Train Time (sec)	1.2255	1.0544	1.0744	1.0986	1.3079	1.1959

The model parameter is used to gauge the performance of various models. After training the Gaussian process regression (GPR), the performance of each feature is compared as shown in Table. The performance of various GPR based models are compared using the subsequent model statistics.RMSE (Root mean square error) is usually positive and its units match the units of the response. Search for smaller value of the RMSE, R-Squared coefficient of determination is usually smaller than or adequate to 1 but always greater than 0. If the model is worse than this constant model, then R-Squared is negative. Search for an R-Squared on the brinkof 1 MSE (Mean squared error). The MSE is that the square of the RMSE, MAE (Mean absolute error) is usually positive and almost like the RMSE, but less sensitive to outliers, Search for smaller value of the MAE.

3.2 Response Surface Optimization

3.2.1 The overlaid contour plot

Overlaid Contour Plot is employed to visually identify the feasible variables for multiple responses for a model. Feasible variable settings for one response might be far away from feasible for a special response. Overlaid contour plots uses to contemplate the reactions at the identical time.

To create an overlaid contour plot, we specified a lower and bound for each response. The various variables in a very model are held at user-specified settings.

The isometric may be a curve that connects plot points, like the fitted response values, which are equal. This can be referred to as the feasible region. Figure Number shows the Overlaid Contour plot showing feasible area for Optimization of Inlet Feed Rate and Reformer Temperature with maximized Methanol Conversion, Hydrogen Formation, and minimized monoxide generation. The overlaid contour plot is as shown in Figure 10.

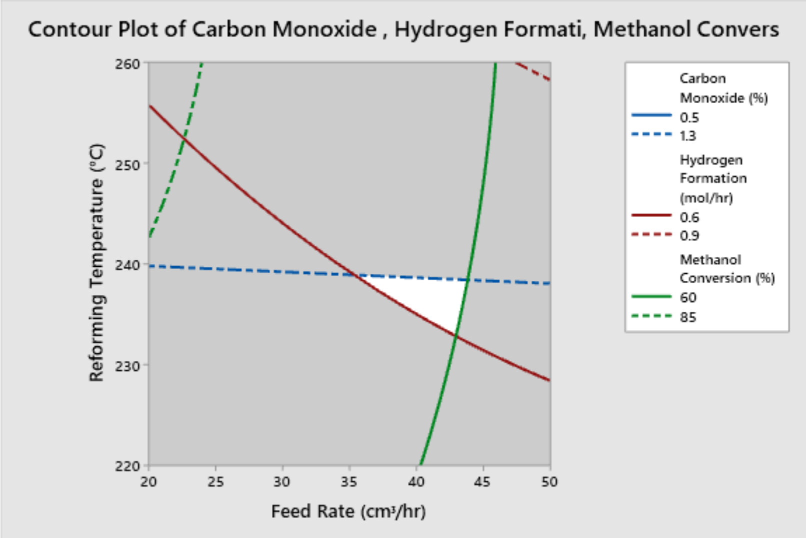


Figure 10: Contour Plot for Feasible Region

3.2.2 Response optimizer

Response Optimizer is utilized to detect the blend of info variable settings that improve one reaction or an assortment of reactions. Minitab computes an ideal arrangement and draws an advancement plot. This intelligent plot permits you to adjust the info variable settings to perform affectability examinations and perhaps enhance the underlying arrangement. The Response Optimizer is used to predict the exact values for Inlet Feed rate and Reformer Temperature, which are 29.3939 cm3/hr and 239.78°C. The graph of optimized values is shown in figure 11.

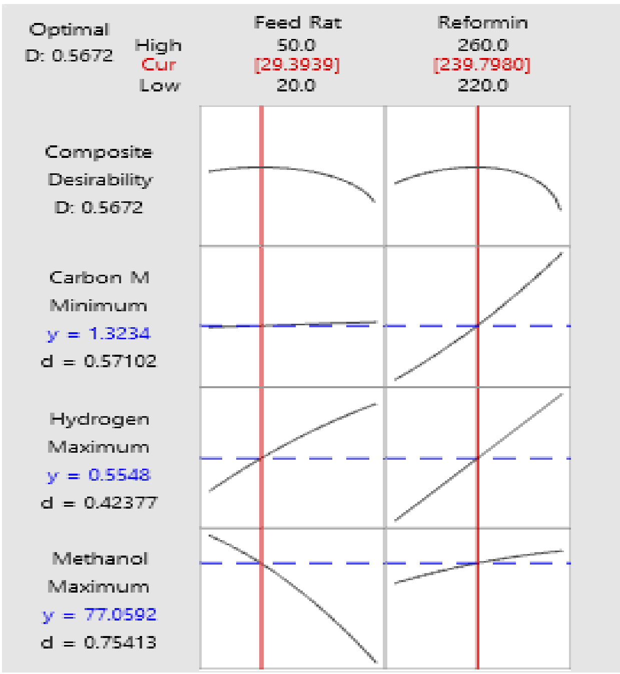


Figure 11: Optimized Response Curves

4. CONCLUSION

From the above study, the Gaussian Progression Regression is implemented with matern 5/2 and matern 3/2 as kernel on compact methanol steam reformer for prediction of methanol conversion, hydrogen generation, and carbon monoxide formation. The low RMSE values 0.54889 and 0.0035743 are obtained for methanol conversion and hydrogen formation for matern 3/2 kernel, whereas 0.0038477 for carbon monoxide generation for matern 5/2 kernel. The Response Surface Optimization was tested on Methanol Steam Reformer. The optimized inlet feed flow rate of 29.3939cm^3/hr. and reformer temperature of 239.798˚C is been observed for predicted data.

REFERENCES

[1] K. D. Kreuer, "On the development of proton conducting polymer membranes for hydrogen and methanol fuel cells," *J. Memb. Sci.*, vol. 185, no. 1, pp. 29–39, 2001, doi: 10.1016/S0376-7388(00)00632-3.

[2] F. Cells and Y. Pocket, "Cells Shrinking Promise Power in Your Pocket," vol. 296, no. May, 2002.

[3] S. Monyanon, A. Luengnaruemitchai, and S. Pongstabodee, "Optimization of methanol steam reforming over a Au/CuO-CeO 2 catalyst by statistically designed experiments," *Fuel Process. Technol.*, vol. 96, pp. 160–168, 2012, doi: 10.1016/j.fuproc.2011.12.024.

[4] Bamidele Victor Ayodele, Siti Indati Mustapa, May Ali Alsaar," Artificial Intelligence Modelling Approach for the Prediction of CO-Rich Hydrogen Production Rate from Methane Dry Reforming," catalyst