Process optimization of catalytic steam reforming of toluene to hydrogen using response surface methodology (RSM) and artificial neural network-genetic algorithm (ANN-GA)

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Abstract. Catalytic steam reforming of toluene (SRT) over nickel-cobalt supported on modified activated carbon for hydrogen production has been investigated. The center composite design of experiment in response surface methodology (RSM) was initially applied to optimize the catalytic SRT for hydrogen production before being utilized in the model building of the hybrid artificial neural network-genetic algorithm (ANN-GA). The genetic algorithm was carried out over the ANN model to achieve the maximum target response. The process optimization modeling using the best fitness function gave an insight of the optimal operating condition in SRT over the prepared catalyst. The results conferred that maximum hydrogen yield could be obtained at the optimal conditions of 700 °C temperature, 0.034 ml/min feed flow rate, 0.1 g catalyst loading and S/C ratio of 1 by ANN-GA model, and 762 °C temperature, 0.022 ml/min feed flow rate, 0.3 g catalyst loading and S/C ratio of 5.6 by the RSM model. Predicted results from ANN model were in higher agreement with the experimental data at R²=0.95 compared with the RSM model.

1. Introduction

Hydrogen (H₂) has attracted considerable attention as the alternative energy carrier in replacing conventional fossil fuel due to its high conversion efficiency and environmentally friendly. However, major reliance on nonrenewable fossil fuel leaving a large carbon footprint to the H₂ manufacturing processes [1]. With the aim of improving the renewability and economy of hydrogen production, biomass and its derivatives are widely used in generating H₂ in the catalytic reforming process, among which tar are the most promising renewable resources. Tar is the unavoidable carbonaceous byproduct from the thermal conversion of biomass which consist of a mixture of polycyclic aromatic hydrocarbons (such as toluene, naphthalene and benzene). Tar deposition lowers gasification performance and upsurge the process maintenance cost due to serious hazards in the process equipment of downstream processes as well as catalyst deactivation [2]. Therefore, removal of tar is very desirable. Among available tar removal methods, catalytic steam reforming is the most effective technique for the removal of tar compared to other methods, such as thermal cracking and biochemical conversion. This is because catalytic steam reforming is able to remove tar effectively and concurrently convert tar to produce valuable H₂ rich gas. One of the drawbacks of thermal cracking is that it requires high energy consumption and produces soot. On the other hand, despite of the capability of biochemical conversion
method in tar removal, it involves limited sources of feedstock (rich in starch or sugar) and have lower rate of tar conversion compared to other tar removal methods [3, 4].

Toluene was used in this study as the tar model compound because it represents as one of the major tar species as well as a stable aromatic structure [2, 5]. Hence, toluene steam reforming was chosen as a model reaction to have a better understanding of tars destruction. In catalytic steam reforming of toluene (SRT) for H₂ generation, other than catalytic performance, another important criterion to be considered is the reforming parameters that has a direct influence in achieving maximum result of H₂ yield. The important parameters in SRT include temperature, feed flow rate, catalyst weight and steam-to-carbon (S/C) ratio. It is anticipated that the predictive modeling and optimization will give an inexpensive and time-efficient approach for the experimental study.

Recently, the response surface methodology (RSM) and hybrid artificial neural network-genetic algorithm (ANN-GA) approaches were widely used for process modeling [6-9]. RSM is a collection of mathematical and statistical technique that is utilized for modeling, analysis and optimization in which the responses are influenced by several variables [10]. It is considered as an economical and effective method of optimization because it reduces the experiments to a fairly low number. An artificial neural network (ANN) is a reliable tool exploited for the prediction of experimental data. It has the capability to use the computational power using parallel processing networks to control the complex relationships between input and output variables or responses together with the ability of learning and generalization [11]. ANN has been extensively used in the prediction of non-linear and complex system data due to its accuracy, precision, time and low cost. The ANN structures are organized based on the biological neuron of a human brain. These networks are designed in form of connecting layers which are connected to one another by the connection known as nodes [12]. The genetic algorithms (GA) are adaptive heuristic search algorithms that were developed based on the evolutionary ideas of natural selection and genetic. It belongs to the greater class of evolutionary algorithms with nature-inspired metaheuristic that carried out stochastic transformations such as inheritance, mutation, selection and crossover, in order to generate solutions to optimization problems. The selection operator selects the elements from current generation for transition according to its fitness values. Mutation operator is then applied to the current element itself to create a new one, while crossover operator imitates biological recombination between elements. The prediction performance and generalization rely on the training of network [13]. Mondal et al. [14] reported that the RSM model is constricted to the second-order polynomial regression resulting in lower predictive capability than ANN model in optimization modeling. High predictability of ANN-GA model may be attributed to its universal ability to learn from observation and draw conclusion through generalization and predictive modeling behavior of the complex nonlinearity of a system [6, 15]. Hence, the comparison assessment between the two models is conducted in this study to investigate the suitability of different optimization models in terms of prediction accuracy and efficiency of these models. According to our best knowledge, very few studies have been reported on the utilization of RSM and hybrid ANN-GA in steam reforming for the hydrogen generation [11, 16-18].

The objective of this paper is to compare two optimization methods; RSM and ANN-GA, in the SRT for the production of H₂. RSM and ANN approaches were employed to predict the relationship between the independent variables and the responses. The accuracy of the predicted data obtained from RSM and ANN-GA models were investigated and the overall prediction capability was also examined.

2. Experimental

2.1. Materials and methods

The chemicals used in synthesizing the catalyst are cobalt (II) nitrate hexahydrate (98%, Sigma-Aldrich) and nickel (II) nitrate hexahydrate (98%, Mérck) and hydrogen peroxide (H₂O₂) (30%, Mérck). The palm kernel shell-derived activated carbon (AC) was purchased from Multi Filter Sdn. Bhd. (Malaysia). Gas cylinders of Nitrogen and Air (99.995% purity) were purchased from Mega Mount Industrial Gases Sdn. Bhd. (Malaysia). Analytical toluene (98%, QRëc) and metal nitrates were used as received.
2.2. Catalyst preparation and steam reforming of toluene

The nickel-cobalt supported on H₂O₂-modified AC catalyst used in this research were prepared. The AC support was modified using H₂O₂-aging method by immersing AC particles (100 μm) for 6h (10ml/g of AC) before it is thoroughly washed and dried overnight at 110 °C. Consequently, the modified-AC supported metal catalyst was prepared via wet impregnation with 10 wt.% loading of each metal and calcination for 4h at 500 °C. The synthesized catalyst was subjected to the catalytic performance in SRT.

Catalytic test was carried out using stainless steel catalytic fixed bed reactor of internal diameter of 13 mm and reactor length of 400 mm placed in a vertical tube furnace (Carbolite MTF 10/15/130, Germany) in a continuous flow system. The reactor temperature was maintained using a programmable temperature controller. The reactants of toluene and water were fed using syringe pump (A99-E Syringe Pump, Razel® Scientific Instrument) and HPLC pump (Series I HPLC Pump, Scientific Instrument), respectively, into an evaporator operated at 150 °C. Nitrogen gas was used as carrier gas with constant flow rate of 15 ml/min controlled by mass flow controller (Alicat Scientific, USA). Then, product gas was analyzed using gas chromatograph (GC 6890N) equipped with a flame ionization detector (FID) and thermal conductivity detector (TCD) using Agilent GS-GasPro (Agilent, 60m x 0.32mm ID) and HP-Plot Q (Agilent, 40m x 0.53mm ID, 40μm) capillary column, respectively. The GC peaks determination and calculation of product gas composition were conducted by the standardization of GC peaks of sample to the NOX Premium standard gas supplied by the Leeden National Oxygen Ltd. Total flow rate of product gas was measured using a digital flow meter Model DFM-04 (PCI Analytics). The H₂ yield (Y₇₈) was monitored as response and calculated using equation (1):

\[ Y_{H_2} (\%) = \frac{F_{H_2}^{out}}{18 \times F_{Toluene}^{in}} \times 100 \]  

(1)

Stoichiometric ratio of water (H₂O) to toluene (C₇H₈) was established according to equation (2), considering SRT and water gas shift reactions were also involved as in equation (3) and (4) [19, 20].

\[ \text{C}_7\text{H}_8 + 14\text{H}_2\text{O} \rightarrow 7\text{CO}_2 + 18\text{H}_2 \]  

(2)

\[ \text{C}_7\text{H}_8 + 7\text{H}_2\text{O} \rightarrow 7\text{CO} + 11\text{H}_2 \]  

(3)

\[ \text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2 \]  

(4)

2.3. Response surface methodology (RSM)

The relationship between the steam reforming parameters and response were conducted based on the sequential statistical central composite experimental design (CCD). A five-level-four-factor central design was employed generating twenty-six (26) runs of experiment. The factors investigated in this study are: temperature (500-900 °C), feed flow rate (0.006-0.034 ml/min), catalyst loading (0.1-0.5 g) and steam-to-carbon (S/C) molar ratio (1-9). These data are coded as X₁, X₂, X₃ and X₄, accordingly. The variables were coded at five levels (-1(α), -1, 0, +1, +2(α)) to achieve the optimized conditions for the maximum percentage of Y₁₁₂ as listed in Table 1. Experimental data obtained was analysed using RSM software that were fitted in a second-order polynomial equation, as in equation (5) [21].

\[ Y = \beta_0 + \sum_{j=1}^{k} \beta_j X_j + \sum_{j=1}^{k} \sum_{i=j+1}^{k} \beta_{ij} X_i X_j + e \]  

(5)

where Y is the variable of response; β₀, the model intercept, βᵢ, βᵢᵢ, βᵢⱼ, are the linear, quadratic and interaction regression coefficients, Xᵢ and Xⱼ are the independent variables; and e is the error term. The linear coefficients and the cross-products are the significant model terms while the effects of the factors on the percentage of hydrogen yield are shown in the 3D representations. The quality of the fit of the model was evaluated using analysis of variance (ANOVA) by applying the sum of squares error (SSE), probability value (t-values), general probability (p-values) and correlation coefficient (R²) [22].
Table 1. Experimental parameters with the value for each level and response.

| Variable                     | Symbols | Level (Coded) |                |                |                |                |
|------------------------------|---------|---------------|----------------|----------------|----------------|----------------|
| Temperature (°C)             | X<sub>1</sub> | Lowest        | -α             | 500            | 600            | 700            | 800            | 900            |
|                              |         | Low           | -1             |                |                |                |                |                |
|                              |         | Center        | 0              |                |                |                |                |                |
|                              |         | High          | 1              |                |                |                |                |                |
|                              |         | Highest       | +α             |                |                |                |                |                |
| Feed Flow Rate (ml/min)      | X<sub>2</sub> | 0.007         | 0.013          | 0.020          | 0.027          | 0.033          |
| Catalyst Weight (g)         | X<sub>3</sub> | 0.1           | 0.2            | 0.3            | 0.4            | 0.5            |
| S:C Molar Ratio              | X<sub>4</sub> | 1             | 3              | 5              | 7              | 9              |

2.4. **Artificial Neural Network (ANN)-Genetic Algorithm (GA)**

ANN is an empirical modeling technique that was utilized in the prediction of experimental results using the experimental operating parameters. The operating parameters were used as the inputs while the experimental results as the output of the model. The first layer is the “input layer”, the second layer being the “hidden layer” and the third layer is the “output layer”, where each layer has the information stored in “nodes” or neurons. Each node in the input layer denotes the value of one independent variable whereas the output nodes specify the dependent variables. As we have chosen the reaction temperature, feed flow rate, catalyst weight and S/C ratio as the independent variables, and Y<sub>H2</sub> as dependent variable, architecture with four input neurons and one output neuron are the chosen network for the single objective optimization in this study. A fully-connected three-layer feed forward multi-layer perceptron ANN model has been used to predict the yield of hydrogen from catalytic SRT for the training of 20 neurons in the hidden layer. In this type of networks, the involved data was constantly flow in a forward direction only from input layer to output layer in which the activation function approximates the biases and weights of the network by applying learning algorithm. The output from input layer then becomes an input to the hidden layer which consequently producing another output layer to become the input for the output layer [23]. This output is identified as the predicted results. In this study, Levenberg-Marquardt (LM) has been used in the modeling of hydrogen production via SRT to achieve the best performance. LM is the fastest algorithm used for the training of neural network since it has a memory reduction feature in the case of a large dataset. The calculated network error was compared with the output continuously until the network reached the minimum error by adjusting the weights and biases. The ANN performance was measured by the mean square error (MSE) as shown in equation (6) [24].

\[
MSE = \frac{1}{N} \sum_{i=1}^{N} (Y_{\text{ANN}} - Y_{\text{Exp}})^2
\]

where Y<sub>ANN</sub> is the predicted output from ANN, Y<sub>Exp</sub> is the experimental data and N is number of samples.

In this study, the dataset was divided into three different sets, in which 70% for the training, 15% for the testing and 15% for the validation of network. The optimal structure of neural network was chosen by using the trial and error method. The number of neurons of hidden layer was achieved by the iteration of network for the minimum mean squared error value (MSE). The selection of the number of neurons is considered as an important step in the development of neural network. This is due to the smaller number of neurons may provide the network an anticipated error whereas the high number of neurons may cause an over-fitting of network. Then, the training and validation-test data were selected randomly from the available sample data. The details of ANN model parameters are listed in Table 2.

Genetic algorithm in Optimization Toolbox (ver. 7.1) of MATLAB software was used to generates the ‘best fitness plot’ for Y<sub>H2</sub> using the genetic algorithm, ‘ga’ function [25]. MATLAB’s ‘ga’ function employs a kind of controlled elitist genetic algorithm that assigns fitness scaling and ranks individuals in objective function space based on the degree of nondomination or dominance depth. Elitist selection mechanism highlights the current best solutions in the subsequent generations without using any operators to them. The controlled elitism that were employed in the function sustains a balance between exploitation and exploration of the objective function space.
The variations of the SRT parameters (in actual coded) and experimental results are given in Table 3. To estimate the optimum $Y_{H2}$ value, the Statistica 8.0 (StatSoft, Inc., Tulsa, USA) software and MATLAB 8.4 2014b™ software was used for the RSM and ANN-GA modeling, respectively.

| No. | Items                      | Specifications               |
|-----|----------------------------|------------------------------|
| 1   | Type of Network            | Feed Forward Neural Network (FFNN) |
| 2   | Training Algorithm         | Levenberg-Marquardt (LM)     |
| 3   | Performance Function       | Mean Square Error (MSE)      |
| 4   | Data Division              | Random                       |
| 5   | Number of Input Layer      | 4                            |
| 6   | Number of Hidden Layer     | 1                            |
| 7   | Number of Output Layer     | 1                            |
| 8   | Number of Hidden Neurons   | 20                           |
| 9   | Learning Cycle (Number of Epochs) | 1000                      |

### Table 2. ANN model parameters.

### Table 3. Experimental design with their experimental and predicted value from RSM and ANN-GA.

| Run | $X_1$ | $X_2$ | $X_3$ | $X_4$ | Experimental | Predicted RSM | Predicted ANN-GA |
|-----|-------|-------|-------|-------|--------------|---------------|------------------|
| 1   | 600   | 0.013 | 0.2   | 3     | 60.42        | 55.62         | 61.56            |
| 2   | 600   | 0.013 | 0.2   | 7     | 64.37        | 60.88         | 62.82            |
| 3   | 600   | 0.013 | 0.4   | 3     | 67.84        | 63.60         | 63.71            |
| 4   | 600   | 0.013 | 0.4   | 7     | 70.33        | 67.72         | 62.96            |
| 5   | 600   | 0.027 | 0.2   | 3     | 55.20        | 53.12         | 75.23            |
| 6   | 600   | 0.027 | 0.2   | 7     | 60.71        | 59.75         | 54.13            |
| 7   | 600   | 0.027 | 0.4   | 3     | 61.16        | 55.82         | 62.96            |
| 8   | 600   | 0.027 | 0.4   | 7     | 58.63        | 61.32         | 64.73            |
| 9   | 800   | 0.013 | 0.2   | 3     | 72.27        | 71.54         | 68.26            |
| 10  | 800   | 0.013 | 0.2   | 7     | 68.14        | 71.18         | 65.23            |
| 11  | 800   | 0.013 | 0.4   | 3     | 80.94        | 79.60         | 79.59            |
| 12  | 800   | 0.013 | 0.4   | 7     | 74.07        | 78.12         | 94.50            |
| 13  | 800   | 0.027 | 0.2   | 3     | 78.43        | 78.73         | 95.15            |
| 14  | 800   | 0.027 | 0.2   | 7     | 73.55        | 79.75         | 70.88            |
| 15  | 800   | 0.027 | 0.4   | 3     | 76.08        | 81.53         | 81.77            |
| 16  | 800   | 0.027 | 0.4   | 7     | 78.92        | 81.41         | 75.88            |
| 17  | 500   | 0.020 | 0.3   | 5     | 24.26        | 34.50         | 37.50            |
| 18  | 900   | 0.020 | 0.3   | 5     | 80.40        | 70.50         | 75.94            |
| 19  | 700   | 0.006 | 0.3   | 5     | 69.00        | 73.89         | 64.56            |
| 20  | 700   | 0.034 | 0.3   | 5     | 79.22        | 74.68         | 69.15            |
| 21  | 700   | 0.020 | 0.1   | 5     | 63.73        | 64.82         | 73.59            |
| 22  | 700   | 0.020 | 0.5   | 5     | 75.19        | 74.45         | 74.38            |
| 23  | 700   | 0.020 | 0.3   | 1     | 69.72        | 82.97         | 82.84            |
| 24  | 700   | 0.020 | 0.3   | 9     | 86.96        | 81.08         | 75.99            |
| 25  | 700   | 0.020 | 0.3   | 5     | 82.07        | 82.97         | 76.08            |
| 26  | 700   | 0.020 | 0.3   | 5     | 83.86        | 82.97         | 76.08            |

### 3.1. RSM regression modeling and analysis of variance (ANOVA)

The regression models for $Y_{H2}$ ($Y_1$) is shown in equation (7). All the models fitted well with the observed and predicted values. The coefficient of determination ($R^2$) is acceptable (>0.85), with 0.87 of variability in the response. High $R^2$ values indicated that the obtained model gave good estimation of response within the studied range. ANOVA was employed to validate the significance of model. Analysis was set with a significance level of 5% and confidence level of 95%. The Fischer F-test was used to verify the adequacy of model. Greater F-value shows that the factors have sufficiently elucidated the variation in data. The F value from ANOVA model is 5.12 implying that the model was significant. There were
only 0.005% chance that the model’s value could occur due to noise. The calculated value should be higher than $F_{\text{tabulated}}$ to reject the null hypothesis, $H_0$. Next, the student’s t-test and p-values were used to understand the interactions between factors and to determine the significance of each coefficient. First order temperature factor was the main contributor for $Y_{\text{H}_2}$. Linear term of temperature was the highest significant for $Y_{\text{H}_2}$ where the p-value is 0.000053. The other quadratic and interaction factors were considered less significant since their p-values were larger than 0.05.

$$Y = -401.4 + 1.1X_1 - 315.5X_2 + 175.2X_3 + 11.8X_4 - 0.0X_1^2 - 44309.9X_2^2 - 111.4X_3^2 - 0.8X_4^2$$
$$+ 3.5X_1X_2 - 0.1X_1X_3 + 0.0X_1X_4 + 490.8X_2X_3 - 94.2X_2X_4 - 1.4X_3X_4$$

(7)

Three-dimensional (3D) response surface plot. The 3D response surface plots were shown to demonstrate the interaction effects between the independent variables and responses. These plots were drawn by varying two variables while the other variable remained at zero level. The surface plot confined in the smallest eclipse of the contour plot specifies the maximum predicted values. Figure 1 elucidates the response surface plots for $Y_{\text{H}_2}$. Response plots for temperature and feed flow rate as well as temperature and catalyst loading has displayed strong interactions for $Y_{\text{H}_2}$.

![3D response surface plots](image)

**Figure 1.** 3D response surface plot for $Y_{\text{H}_2}$ and (a) temperature vs feed flow rate, (b) temperature vs catalyst loading, (c) temperature vs S/C ratio, and (d) catalyst loading vs feed flow rate, (e) S/C ratio vs feed flow rate and (f) S/C ratio vs catalyst loading.

### 3.2. ANN-GA modeling

In this paper, the MATLAB 2014b™ (The Mathworks Inc.) was used to develop the codes by designing a multiple-input and single-output neural network for the prediction of $Y_{\text{H}_2}$. The obtained experimental data from the Design of Experiments (DOE) software of RSM are used to develop the FFNN model for the catalytic SRT. Figure 2 illustrates the selected ANN architecture (4-20-1) used in this study.

Prior the training of the network, the hidden neurons were selected and tested for the ANN model where the number of neurons in the hidden layer was selected based on the minimum MSE value. The error minimization within the network involves an appropriate selection of the number of neurons in the hidden layer. In order to obtain the minimum MSE of the training network, the number of hidden neurons was tested for the corresponding MSE starting from the lowest value. Consequently, this process
will yield the optimum neurons at the lower MSE value. This study uses the ANN model that was trained and tested from 1 to 20 number of neurons. The trained network with 14 hidden neurons is found to yield the minimum value of MSE of 82.12 that occurred at the 5th network for $Y_{\text{H}_2}$.

A MATLAB function using the ANN model as the input was coded to create a fitness function for the GA optimization problem[26]. The hydrogen yield component to be maximized was negated in the vector valued fitness function separately since ‘ga’ minimizes all the objectives. Experimental ranges were set as bounds on the four input variables and fifty individuals within the bounds were chosen in the initial population. Then, the algorithm options were set as follows.

- Selection function: Stochastic uniform
- Crossover function: Constraint dependent with crossover fraction set at 0.8
- Mutation function: Constraint dependent mutation function
- Direction for migration: Forward with migration fraction set at 0.2
- Nonlinear constrain algorithm: Augmented Lagrangian
- Population size: 50

The weighted average change in the fitness function value over 100 generations was used as the stopping criteria for the algorithm. The parameter optimization using GA approach were carried out to generate a set of best fitness points. Best fitness plots can assist the process operator to fix the input control variables to achieve the locally optimum points of selected operating parameters with respect to $Y_{\text{H}_2}$. The optimized best fitness plots for $Y_{\text{H}_2}$ were achieved after 311 iterations, as shown in Figure 3.

![Figure 2. ANN model structure for the prediction of hydrogen yield.](image)

![Figure 3. Best fitness plot for $Y_{\text{H}_2}$ obtained from ANN-GA model.](image)
3.3. Comparison of RSM and ANN-GA model

It was observed that the experimental and simulated values having a very minor difference in which determined from the errors. In this study, the performance of constructed RSM and ANN models were evaluated using the root mean square error (RMSE) and coefficient of determination (R²), as in equation (8) and (9). These errors value gives the information of the predicted values in good agreement with experimental values where highest R² value will be obtained for the lowest error.

\[
RMSE = \left( \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \right)^{1/2}, \tag{8}
\]

\[
R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}. \tag{9}
\]

In comparison of R² and RMSE value, it is observed that both RSM and ANN-GA fitted well with the experimental data as listed in Table 4. ANN model gives higher R² and lower RMSE value indicating that the ANN model has higher predictive accuracy and suitability than RSM model [8, 27]. The predominance of ANN modeling over RSM as a predictive modeling tool coincides with current studies on H₂ production reported by Ayodele et al. [28], Jha et al. [29] and Azaman et al. [30], who employs the RSM and ANN for the modeling of H₂ production. This is attributed by the universal ability to estimate non-linearity of the system while RSM is only constrained to second order polynomial. Hence, this shows that the developed ANN-GA model is suitable to represent the yield of hydrogen. Subsequently, the Y₁₁₂ was predicted at the optimum operating parameters for both RSM and ANN-GA model. This result coincides with previous report by Ayodele and coworkers where the experimental data based on its temperature resulted in high Y₁₁₂ which may attributed by the Arrhenius behavior for temperature-dependent chemical reaction [28]. The predicted response obtained from RSM and ANN models as well as the experimental results for each experimental run were also listed as in Table 3.

Table 4. Optimum parameters, predicted response and statistical parameters for Y₁₁₂ using RSM and ANN model.

| Response Model | Optimum parameter | X₁ | X₂ | X₃ | X₄ | X₅ | Y₁₁₂ (Yᵢ) |
|----------------|-------------------|----|----|----|----|----|------------|
| R²             | 0.95              | 5.6| 0.3 | 0.034 | 0.1 | 700 | 762         |
| RMSE           | 4.09              | 6.92| 0.87| 0.022 | 0.3 | 86.3%| 93.7%       |

4. Conclusion

This study provides the comparative assessment of the RSM and ANN-GA optimization models in the catalytic steam reforming of toluene using nickel-cobalt supported on modified-AC catalyst. The response surface plots display the increase in temperature as the strong determinant in achieving maximum Y₁₁₂. The experimental data and the predicted values of the selected response for both RSM and ANN models demonstrate the ability of the models to predict the experimental data based on its good correlation with the validation experiments. Comparative assessment of the RSM and ANN-GA models are carried out using statistical parameters of regression coefficient (R²) and root mean squared error (RMSE). The predictive values derived from ANN-GA model exhibit superior predictive capability due to its higher R² and RMSE values of 0.95 and 4.09, respectively, compared to the RSM model with 0.87 and 6.92, respectively. Moreover, the optimal conditions and maximum H₂ yield are determined by both models. The RSM model reveals that the optimal parameters of the studied variables
are temperature of 762 °C, a feed flow rate of 0.022 ml/min, catalyst loading of 0.3 g and S/C ratio of 5.6 with maximum predicted H\textsubscript{2} yield of 86.3%. The ANN-GA model confer that the optimal parameter conditions are temperature of 700 °C, feed flow rate of 0.034 ml/min, catalyst loading of 0.1 g and S/C ratio of 1 with maximum predicted H\textsubscript{2} yield of 93.7%.

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