

# Bio-Metal Organic Framework based on Chromium Citric Acid for Automatic Adsorption of CO<sub>2</sub> Capture with Multi-Objective Optimization Artificial Intelligence Methods

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## Abstract

Carbon dioxide gas is one of the factors and contributors to climate change. However it also can be used to make renewable energy by using CO<sub>2</sub> Capture and Storage. In this study, we required a renewable metal framework composite that where biological metal organic framework (bio-MOF) is required. Citric acid also plays a crucial role in this study, citric acid is very practical because it's obtained very easily and it's non-toxic. This study involved prediction and optimization by using the combination of Artificial Neural Network (ANN) and Design expert. The two inputs are temperature and pressures, while the outcome are CO<sub>2</sub> uptakes and heat adsorption. In addition to this the multiobjective genetic algorithm (MOGA) approach is also used to maximize optimization for CO<sub>2</sub> uptakes and heat adsorption. The CO<sub>2</sub> uptakes and heat adsorption coincide satisfactory with the values predicted by ANN with high validity of R=0.99. In this research, we look at how bio-MOFs may be used to extract CO<sub>2</sub> and review the principles of CO<sub>2</sub> adsorption and industrial system requirements. We also examine both experimental and theoretical studies of the structural factors of bio-MOFs that impact CO<sub>2</sub> adsorption efficiency, heat of adsorption, and selectivity.

**Keywords :** Carbon dioxide , biological metal organic framework, Artificial Neural Network, Citric acid

## 1. Introduction

The impact of climate change is one of the most complicated and significant challenges facing today's society. [Over the next 40 years, the global population will grow from 7 to 9 billion.](#) Fossil fuels, coal gas and oil supply 80% of the world's energy needs. As a result, releasing enormous quantities of CO<sub>2</sub>, which is the principal driver of global warming. [Today's atmospheric CO<sub>2</sub> concentration reaches 410 ppm. It is likely to rise further and surpass 550 ppm by 2050.](#) A solution to this is to have greater energy efficiency, use renewable energy and CO<sub>2</sub> Capture and Storage (CCS). [CCS is one sustainable energy technology that has emerged as a viable answer to alleviate climate change and global warming on time.](#)

Renewable energy is common and accessible but it is hard to implement therefore, another alternative to reducing climate change is carbon capture and storage (CCS). "Carbon capture and storage is going to be the only effective way we have in the short term to prevent carbon emissions from the steel industry, cement manufacture and many other processes", says Professor Stuart of Edinburgh University.

CCS includes the process of absorption, adsorption, cryogenic, and membrane separation. The most advanced CO<sub>2</sub> capture technique is absorption, which uses liquid amine scrubbing to separate CO<sub>2</sub>, H<sub>2</sub> and CH<sub>4</sub> to improve natural gas quality. The most used amine solutions are Methyldiethanolamine (MDEA), Diethanolamine (DEA), Aminoethoxy Ethanol, and Diisopropanolamine (DIPA). However, amine scrubbing produces waste disposal with volatile degradation compounds which have been studied to potentially harm human health and the environment. Moreover, it also requires high energy for regeneration, and is vulnerable to material corrosion. It also degrades amines to toxic chemicals such as ammonia. As a result, researchers are concentrating on the development of adsorption technology that promises the possibility for effective CO<sub>2</sub> removal from high dilution in the flue gas while also using little energy for regeneration. [Adsorption process is the process in which the one or more component of a gas or liquid stream is adsorbed on the surface of a solid adsorbent and a separation is accomplished.](#) Because CO<sub>2</sub> adsorption is an effective separation technique that needs low energy and financial

commitment, porous adsorbents may be the solution to these challenges. Global zeolites, activated carbon, and silica gel, metal organic frameworks (MOFs) are examples of porous materials used for CCS.

For this research, we will be using MOFs as our porous material. Because of their hybrid origin, MOFs have a unique chemical structure which consist of metal centers and organic ligands. Unlike amines, MOFs are more thermally stable at temperatures as high as 200°C, have lower energy requirements and enhanced stability. [MOFs feature](#) a number of distinguishing qualities and therefore have developed as next-generation adsorbent materials. They are appealing as gas storage materials due to their extremely large surface areas, high porosity, readily regulated pore diameters, outstanding thermal and chemical stability, quick kinetics, and moisture resistance. Bio-MOF, specifically, would be the type of MOF we will use. The demand for ecologically friendly and cost-effective technologies to counteract extreme climate change has accelerated the development of renewable and porous materials based on green chemistry concepts such as renewability and recyclability. Biological MOFs, also known as bio-MOFs, are made up of physiologically and ecologically suitable metal ions and biomolecular ligands therefore would be the best choice for our porous material.

## 2. Methodology

This study is divided into three sections. The first section of the study focuses on the analysis of bio-MOFs for CO<sub>2</sub> adsorption. Furthermore, in the second phase of the research, the researchers investigated the predictions of CO<sub>2</sub> uptake, heat of adsorption, and CO<sub>2</sub>/N<sub>2</sub> selectivity using neural network modeling, and then continued with artificial neural network optimization using a multiobjective genetic algorithm approach.

### 2.1 Materials

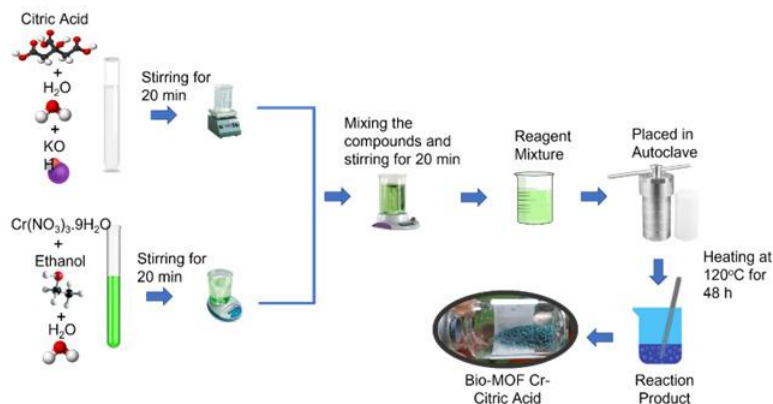
Merck supplied Chromium Nitrate nonahydrate (CrH<sub>12</sub>N<sub>3</sub>O<sub>7</sub>) as the metal and citric acid monohydrate (C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>) as the ligand. Merck also provided potassium hydroxide (KOH), ethanol (99.7%) and N, N dimethylformamide (DMF, 99.5%) for the

[In this research, citric acid, C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>, was chosen to be our reagent as it is cost effective, obtained easily and non-toxic. Citric acid is a type of ligand that contains basicity and composed of COOH \(carboxylic acid\) which can absorb CO<sub>2</sub> better compared to other reagents. The presence of citric acid in the synthesis system can improve hydrogen bonding between the triblock copolymer and resin, resulting in more micropores in the final carbon material, which is beneficial for CO<sub>2</sub> adsorption.](#) Our objectives for this research are to investigate the CO<sub>2</sub> uptakes, to analyze the energy needed between bio-MOF and citric acid, and to design automatic adsorption carbon capture. Then, we will find the optimization parameters in the adsorption process which is the temperature and the pressure operation in the flue gas as the result of the combustion process. Furthermore, we will be using a method called artificial intelligence with multiobjective genetic algorithm optimization. We hope that this research will pave the way for researchers and practitioners to be able to estimate the high CO<sub>2</sub> uptakes with the concept of a sustainable low-cost of CO<sub>2</sub> capture technology.

purification of Bio-MOF, which were utilized exactly as received. These products are known to be more environmentally friendly than NaOH in adjusting the pH level of the MOF solution.

### 2.2 Bio-MOF Synthesis

This synthesis was carried out using a hydrothermal reaction procedure using the following material mixture: Chromium Nitrate (2.5 g), Citric Acid (2.1 g), Potassium Hydroxide (1.7 g), Ethanol (2.5 mL), and deionized water/Aquabidest (2.5 mL), as shown in **Figure 1**. These components were combined and placed into the stainless steel autoclave's reactor. The autoclave was gradually heated in the oven from room temperature to 120 degree celsius in 30 minutes. After reaching 1200 degrees Celsius, the temperature was kept constant for 48 hours.



**Figure 1** Hydrothermal reaction on Bio-MOF

### 2.3 RSM Predictive Model

In order to figure out the natural relationship amongst the unalike parameters in the experiment from the dependence and interaction between them that were shown through the outcomes of the experiments, Design of Experiment (DoE) is used. Face-centered central complex design with six center points and eight-corner points was used in the DoE analysis intending to enhance the end results. Using the inputs and responses, DoE end results were obtained and a verifiable connection was expanded. In order to obtain the result, DoE end results are then statistically inspected using Response Surface Method (RSM).

RSM is a reliable analysis method for examining multiple inputs and outputs for modeling and optimization. Moreover, it is also a robust analysis technique to survey several inputs and responses for modeling and optimization. The least well known components are used in the RSM analysis, which leads to a more reliable discovery. The input parameters, response, and interaction in the first stage were displayed in a linear equation that was then used in the optimization process of the parameters in the next stage. With RSM, a verifiable linear equation relationship between the input parameters and their responses was improved. The analysis of variance (ANOVA) measures the average squared, sum of squared deviations, and degree of freedom of the model for every single input value. ANOVA was made use of afterwards for optimization through the application of the input parameters and significance of the model to ANOVA on linear equations.

### 2.4 ANN Based Predictive Model

Artificial Neural Network, ANN, effective data-driven modeling tools that are frequently employed for the dynamic modeling and identification of nonlinear systems. This is because of their capacity for universal approximation and flexible structure, which enables them to capture complicated nonlinear behaviors. They are made up of tiny intelligent computing units called neurons that are utilized to represent complex nonlinear systems in accordance with the groupings of input-output data that are readily available. Finding the correlations between the experiment's variables is difficult as there are many conditions that must be met, as well as problematic calculations that consume lots of time. The ability of an artificial neural network to produce specific equations from the data given into it makes it practical for pinning down these links. Artificial neural networks are practical because they reduce costs, time, and work.

In this research study, a multilayer perceptron (MLP) is utilized, meaning it connects the networks in a feed-forward configuration to create the ideal network. MLP is frequently considered as the most effective method for solving nonlinear issues. Rather than multiple layers of neurons, the MLP framework embodies optimized neurons and 3 interconnected layers: input layer, hidden layer, and output layer. The hidden layer is attached to every input layer, consisting of multiple transfer functions related to biological neurons. Last but not least, the output layer presents the projection of the advanced model.

The number of neurons is very noteworthy to find the optimal network size and is often chosen based on trial and error method or a heuristic approach. Deciding and selecting the optimal quantity of neurons is a critical step as a high number of neurons might cause overfitting, in reverse, a lower number of neurons might cause the results to underfit. As stated earlier, to avoid overfitting due to MLP, the input data went through multiple several essential processes: training, validation, and testing. Through synapse adjustments, the training of neurons helps design a prime ANN model, while validation helps oversee the learning curve of neurons. Both processes can only be stopped when the universal Mean Square Error (MSE) in the training stage is higher than the ones used are 70% of the data sets. The other 15% of each data set were employed in the validation and testing process. When data is officially validated, the evolved model is used to trigger experimental data at numerous input conditions.

## 2.5 Genetic Algorithm (GA)

Genetic algorithm was first initiated by John Holland and David Goldberg and its concept has been very present in lots of different areas, showing that it has been properly and nicely designed. In short, genetic algorithms are a group of alike algorithms that draw upon the ideas of Darwinian genetics and evolution. As time flies, genetic algorithm constantly provide satisfactory results.

## 2.6 Multi-objective Optimization

This research uses ANN to understand more deeply about this research's multi-objective optimization. We have gathered several sets of data in advance before conducting this research.

Using MATLAB ANN, we enter the data that we had collected and the software will release prediction results that will then be optimized by genetic algorithm (GA). The optimized results will be considered on whether it has been obtained or not. Nevertheless, if the result isn't optimum, the decision variable's beginning value is once again set, repeated over and over until the appropriate outcome is achieved. The following equations can be used to design a multiobjective optimization:

$$\text{Find } x = (x_i) \forall i = 1, 2, \dots, N_{par} \quad (1)$$

$$\text{Minimizing or maximizing} \quad (2)$$

$$f_i(x) \forall i = 1, 2, \dots, N_{obj} \quad (3)$$

$$g_j(x) = 0 \quad \forall j = 1, 2, \dots, m \quad (4)$$

$$h_k(x) = 0 \quad \forall k = 1, 2, \dots, n \quad (4)$$

GA is unique than any other types of algorithms as it has numerous solutions, rather than a one, single 'current' solution. Multiple stages in the optimization process by multi-objective genetic algorithm is represented in Figure 2.

In order to carry out GA, it is essential to make a number of decisions about how to represent solutions, how to manipulate information and how the population is taken good care of: GA randomly chooses the populations and applies the fitness function. Those individuals with sufficient match values will be chosen to enter the crossover stage, while individuals with low match values will be eliminated. Moreover, individuals who have been selected to the crossover stage will be paired to assemble new individuals who have a combination of information from their parents. Then, the individuals will undergo random mutations and show up as a new population, including their parents. Up until the best result is obtained, this cycle will repeat itself. The optimization process is carried out in MATLAB's optimization toolbox, along with the neural function established during the set up of the artificial neural networks as the fitness function. The constraints of each variable are determined. The optimization parameters are then set until the optimization function is ready to run.

$N_{par}$  is the number of decision variables,  $f_i(x)$  is the objective function, and  $N_{obj}$  is the total number of objective functions where  $x$  is the vector of choice variables.  $g_j(x)$  and  $h_k(x)$ , respectively, stand for the fairness and unfairness conditions. The quantity of fairness and unfairness constraints, respectively, is represented by  $m$  and  $n$ .

## 3. Results & Discussion

### 3.1 Result of synthesis Bio-MOF citric acid

[The Bio-MOF Citric Acid was fabricated by hydrothermal reaction using the eco-friendly solvents Aquabidest and potassium hydroxide \(KOH\)](#) used to balance the pH of the solution. After stirring each separate mixture, the two solutions are reacted again by stirring, then placed in an autoclave. It is then heated in the oven at 120 degrees celsius for 48 hours, and the BIO-MOF Citric Acid is produced. After heating, the BIO-MOF Citric Acid product has to be cleaned and purified. The purification is done in order to remove any unreacted substances that might be sticking onto the surface of the end product. [The](#)

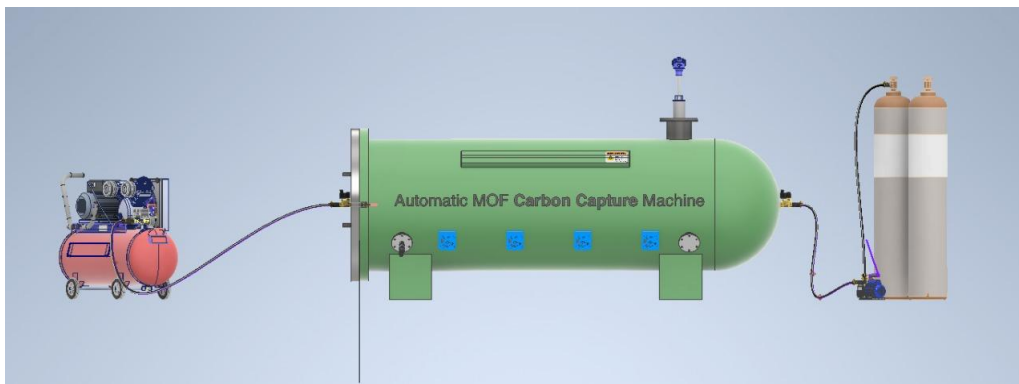
[purification is done by washing the crystals formed in an organic solution, and then rinsing the product with ethanol. This purification process has been proven to be better for crystallinity of the BIO-MOF.](#)

### 3.2 Automatic Adsorption Carbon Capture (Element Peltier)

The device that the BIO-MOF is implemented into is called the Automatic Adsorption Carbon Capture Device. It consists of 3 parts: the compressor, Automatic Adsorption Carbon Capture Vessel, and the gas tanks, which can be seen in **Figure 2**.

The use of the compressor is to facilitate the procedure of gathering CO<sub>2</sub> from around the device. Because of the compressor, air from around the device is being absorbed easily, particularly the CO<sub>2</sub>, therefore making the process more effective. After the CO<sub>2</sub> has been adsorbed, there are element peltiers in the device that are actively regulating the internal temperature of the device. It regulates the internal

temperature to be colder when the CO<sub>2</sub> is being adsorbed using the compressor, therefore making the CO<sub>2</sub> liquid and facilitating it to be reacted with BIO-MOF Citric Acid. It regulates the internal temperature to be hotter when it is about to be transported into the gas tanks, the liquid phase of CO<sub>2</sub> is then heated back into the gas tanks as CO<sub>2</sub> gas. The process of transporting CO<sub>2</sub> gas into the gas tanks is helped with the use of vacuum pumps. As shown in the figure So first, the vessel is being placed in a (preferably) outdoor position where there is an abundant amount of CO<sub>2</sub>. Second, the compressor (on the right) helps the vessel absorb the CO<sub>2</sub> from around it. Next, the element peltiers (the blue devices) on the vessel regulate the internal temperature to be cooler in order to liquify the CO<sub>2</sub> and facilitate it to react with the BIO-MOF Citric Acid. After reaction, the CO<sub>2</sub> is then heated up by the peltiers to convert it back into gaseous form, facilitating the vacuum pump to adsorb the CO<sub>2</sub> into the gas tubes.



**Figure 2** Automatic Adsorption Carbon Capture Device

### 3.3 Design Expert, Model Development, and Verification

Design of Experiment (DoE) was used to figure out the relationship among the different parameters in the experiment from the dependence and interaction between them, which were shown through the outcomes of the experiments. Face-centered central complex design with six center points and eight-corner points was made use of in the DoE analysis intending to improve the outcomes. Using the inputs and responses, DoE outcomes were gained and a verifiable connection was developed. In order to obtain the result, DoE outcomes are then statistically examined using Response Surface Method (RSM).

The variations of desirability and uptake were observed by changing the values of pressure and

temperature. **Table 1** shows the fit summary of heat adsorption analysis response by using Design Expert. Based on **Table 2**, it displays the fit statistics of the final results of standard deviation, mean, and curriculum vitae, respectively. The ANOVA results of Heat Adsorption are seen from **Table 3**. The findings show how the inputs along with their squares and interactions, helps in analyzing and executing the output. In addition, it also demonstrates how these features are critical for assessing the generated model. **Table 3** shows that for Heat Adsorption with a P-value of <0.05, the corresponding F-value for the constructed model is 489.39. Model terms with P-values less than 0.0001 are notable, consequently these are appropriate model terms in this scenario. The results from **Table 3** demonstrate the value of the developed model in optimizing and estimating Heat Adsorption. Eq (1) is the model's representation. The



equation involves the various parameters that affect Heat Adsorption.

$$\text{Heat Adsorption Formula} = -2409.27 + 15.66*A + 0.119384*B + -0.000332085*AB + -0.0244653*A^2 + -4.98065e-07*B^2 \quad (1)$$

The fit summary of heat adsorption analysis response by using Design Expert is demonstrated in **Table 4**. Based on **Table 5**, it displays the fit statistics of the final results of standard deviation, mean, and curriculum vitae, respectively. **Table 6** shows the

ANOVA results to estimate the uptakes with an F-value of 2154.14 and P-value of <0.05. All the p-values present are 0.0001 which is closer to 0, making the model more remarkable. Eq (2) is a representation of a developed model for uptakes estimation.

$$\text{Uptakes Formula} = -15.3589 + 0.0950494*A + 0.00084637*B + -2.44752e-06*AB + -0.000146769*A^2 + -1.51836e-09*B^2 \quad (2)$$

Using normal plots for residuals, the suggested model was tested for acceptability and irregularity of data. A

good model should not follow neither trend nor sequence and the points should be near to a straight line. **Figure 3** portrays the residual plots for the Heat Adsorption. In the report of **Figure 3**, all data points SOMETHING SOMETHING. **Figure 4** shows the residual plot for uptakes response. Data points that exceed the allowed range of  $\pm 3.67$  are considered abnormal. According to **Figure 3b** all data points fall inside this permitted range. Anything outside this range would also be considered abnormal.

Based on **Figure 5**, there are four different parametric studies in which one of them is the optimum temperature for the variable A, B for pressure, and the rest for minimum Heat Adsorption and maximum Uptakes. The main goal of this research is to maximize the value obtained in uptakes with the minimum heat adsorption. The most suitable temperature is 312.635 and pressure is at 2100.104. Bio-MOF Citric Acid Chromium Optimization would work best at 0.175 as its maximum uptakes and 125.821 as its minimum heat adsorption with a desirability of 0.405.

| Source           | Sequential p-value | Lack of Fit p-value | Adjusted R <sup>2</sup> | Predicted R <sup>2</sup> |                  |
|------------------|--------------------|---------------------|-------------------------|--------------------------|------------------|
| Linear           | < 0.0001           |                     | 0.5067                  | 0.4939                   |                  |
| 2FI              | < 0.0001           |                     | 0.8358                  | 0.8291                   |                  |
| <b>Quadratic</b> | <b>&lt; 0.0001</b> |                     | <b>0.9264</b>           | <b>0.9218</b>            | <b>Suggested</b> |
| Cubic            | < 0.0001           |                     | 0.9877                  | 0.9859                   | <b>Aliased</b>   |

**Table 1** Fit Summary of DoE Analysis Response of Heat Adsorption

|           |        |                          |         |
|-----------|--------|--------------------------|---------|
| Std. Dev. | 4.51   | R <sup>2</sup>           | 0.9283  |
| Mean      | 130.00 | Adjusted R <sup>2</sup>  | 0.9264  |
| C.V. (%)  | 3.47   | Predicted R <sup>2</sup> | 0.9218  |
|           |        | Adeq Precision           | 75.3491 |

**Table 2** Fit Statistics of DoE Analysis Response of Heat Adsorption

| Source           | Sum of Squares  | df         | Mean Square    | F-value       | p-value            |
|------------------|-----------------|------------|----------------|---------------|--------------------|
| <b>Model</b>     | <b>49720.63</b> | <b>5</b>   | <b>9944.13</b> | <b>489.39</b> | <b>&lt; 0.0001</b> |
| A-Temp           | 7153.37         | 1          | 7153.37        | 352.05        | < 0.0001           |
| B-p              | 9429.93         | 1          | 9429.93        | 464.08        | < 0.0001           |
| AB               | 4250.00         | 1          | 4250.00        | 209.16        | < 0.0001           |
| A <sup>2</sup>   | 881.03          | 1          | 881.03         | 43.36         | < 0.0001           |
| B <sup>2</sup>   | 4117.33         | 1          | 4117.33        | 202.63        | < 0.0001           |
| <b>Residual</b>  | <b>3840.37</b>  | <b>189</b> | <b>20.32</b>   |               |                    |
| <b>Cor Total</b> | <b>53561.00</b> | <b>194</b> |                |               |                    |

**Table 3** ANOVA Results of Head Adsorption

| Source           | Sequential p-value | Lack of Fit p-value | Adjusted R <sup>2</sup> | Predicted R <sup>2</sup> |                  |
|------------------|--------------------|---------------------|-------------------------|--------------------------|------------------|
| Linear           | < 0.0001           |                     | 0.5971                  | 0.5889                   |                  |
| 2FI              | < 0.0001           |                     | 0.9430                  | 0.9412                   |                  |
| <b>Quadratic</b> | <b>&lt; 0.0001</b> |                     | <b>0.9823</b>           | <b>0.9815</b>            | <b>Suggested</b> |
| Cubic            | < 0.0001           |                     | 0.9997                  | 0.9997                   | <b>Aliased</b>   |

**Table 4** Fit Summary of DoE Analysis Response of Uptakes


|           |        |                          |          |
|-----------|--------|--------------------------|----------|
| Std. Dev. | 0.0125 | R <sup>2</sup>           | 0.9828   |
| Mean      | 0.2000 | Adjusted R <sup>2</sup>  | 0.9823   |
| C.V. (%)  | 6.26   | Predicted R <sup>2</sup> | 0.9815   |
|           |        | Adeq Precision           | 163.3985 |

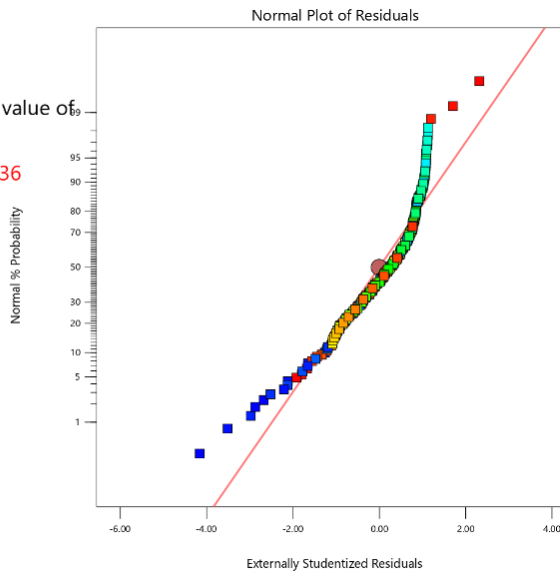
**Table 5** Fit Statistics of DoE Analysis Response of Uptakes

| Source           | Sum of Squares | df         | Mean Square   | F-value        | p-value            |
|------------------|----------------|------------|---------------|----------------|--------------------|
| <b>Model</b>     | <b>1.69</b>    | <b>5</b>   | <b>0.3373</b> | <b>2154.14</b> | <b>&lt; 0.0001</b> |
| A-Temp           | 0.3561         | 1          | 0.3561        | 2274.04        | < 0.0001           |
| B-p              | 0.4979         | 1          | 0.4979        | 3179.93        | < 0.0001           |
| AB               | 0.2309         | 1          | 0.2309        | 1474.43        | < 0.0001           |
| A <sup>2</sup>   | 0.0317         | 1          | 0.0317        | 202.51         | < 0.0001           |
| B <sup>2</sup>   | 0.0383         | 1          | 0.0383        | 244.39         | < 0.0001           |
| <b>Residual</b>  | <b>0.0296</b>  | <b>189</b> | <b>0.0002</b> |                |                    |
| <b>Cor Total</b> | <b>1.72</b>    | <b>194</b> |               |                |                    |

**Table 6** ANOVA Results of Uptakes

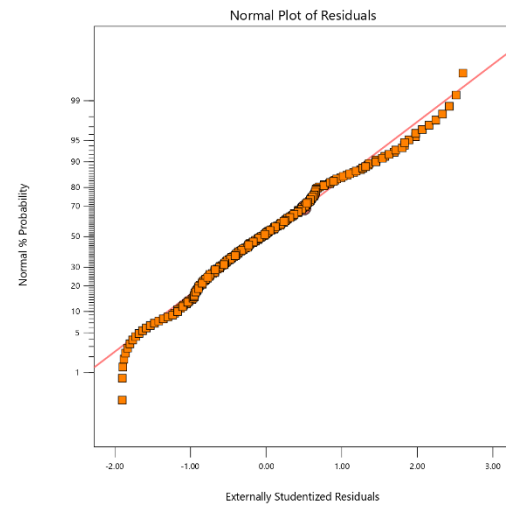
**Hads**

Color points by value of Uptake n:  
0.04  0.36

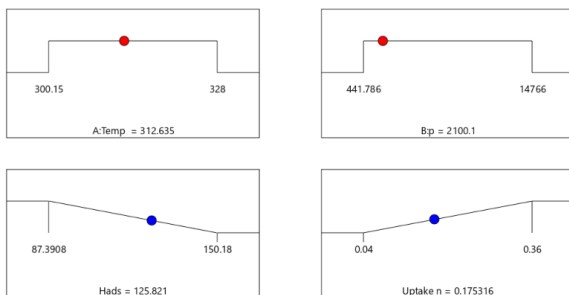


**Figure 3** Normal Plot of Head Adsorption Response

**Uptake n**



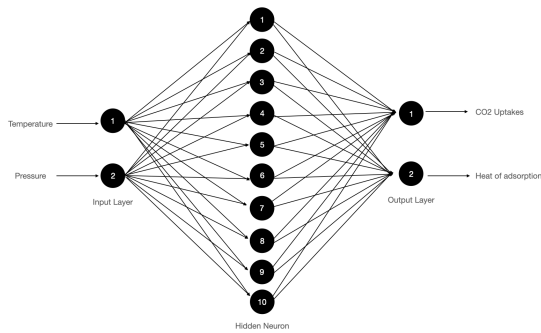
**Figure 4** Normal Plot of Uptakes Response



← **Figure 5** Ramp Function of RSM Optimization

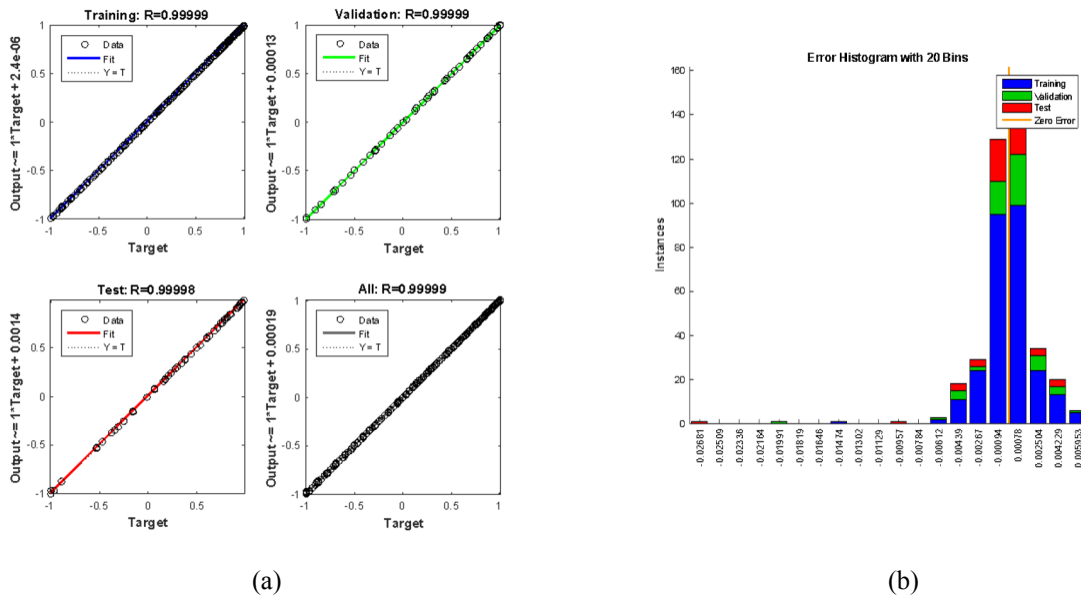
### 3.4 Artificial neural network modeling

In this study, the ANN modeling used consisted of 2 inputs, 1 hidden layer and 10 hidden neurons, and 2 target outputs. The trial-and-error method was used to find the optimal design, and the architecture with the lowest error (RMSE) and best regression coefficient was chosen. **Figure 6** depicts the architecture of the artificial neural network that was designed. The discrepancy between the neural networks's output and the desired data is known as the network error level. By computing the weights to achieve the best weight to employ in the testing phase, the backpropagation algorithm enables neurons to learn new information. To reduce mistakes that may arise during learning, the weights are changed repeatedly. This reverse computing technique can significantly lower the value of the mistake.



**Figure 6** Architecture of ANN modeling

Root mean square error (RMSE), mean absolute error (MAE), and mean bias error (MBE) were used to determine the error for each neuron and each data category. The closer the regression of coefficient (R) to 1 is, the more accurate the trendline as the R-value is 0.99. It also shows that it is touching every dot on the graph. The regression coefficient (R) values for the trendlines in the data are  $R = 0.99$  for the training data,  $R = 0.99$  for the validation data, and  $R = 0.99$  for the testing data and  $R = 0.99$  for all data combined, as illustrated in **Figure 7a**. The ANN regression shows several correlation coefficients and comparisons between regression model and ANN during training validation, and testing. **Figure 7b** illustrates the error histogram, training performance, and training state, respectively. The error histogram is a histogram of the differences between the target and predicted values after the feedforward neural network has been trained. These error numbers show how the expected and goal values differ. The performance graph depicts the network's best validation performance. The variation in the gradient coefficient with respect to the number of epochs is the training state.



**Figure 7** (a) ANN regression data (b) error histogram of network



### 3.5 MOGA Optimization

#### 3.5.1 DoE MOGA Optimization

DoE MOGA analysis was polished using MATLAB software, obtaining Pareto graphs. The optimization process was implemented using the equation that has originated from DoE, respectively Eq. (8)-(10). These objective values are maximized to get desired carbon adsorption towards bio-mof citric acid chromium. The input range values of pressure and temperature were determined based on the previous experimental data. The results of the optimization with the DoE equation can be seen in Figure 8. The Pareto graph obtained here shows that the Co2 uptake and heat adsorption maximum values reached to 26% and 24%

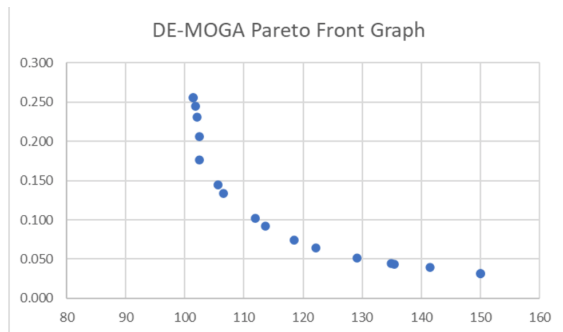


Figure 8 DoE MOGA Optimization

with the minimum optimal values for are 3% and 4% respectively. The optimum value generated by MOGA is still in the same range as the optimization with DoE as described in Table 7.

| No | Temp    | p         | Hads    | Uptake n | Desirability |
|----|---------|-----------|---------|----------|--------------|
| 1  | 312.635 | 2100.104  | 125.821 | 0.175    | 0.405        |
| 2  | 312.677 | 2101.008  | 125.819 | 0.175    | 0.405        |
| 3  | 312.535 | 2098.577  | 125.833 | 0.175    | 0.405        |
| 4  | 312.702 | 2100.503  | 125.803 | 0.175    | 0.405        |
| 5  | 328.000 | 14765.949 | 140.993 | 0.340    | 0.370        |
| 6  | 328.000 | 9074.043  | 149.038 | 0.298    | 0.121        |

Table 7 Optimization Results Received

Table 7 Optimal Results of DoE MOGA Optimization

#### 3.5.2 ANN MOGA Optimization

The developed network function is found to be accurate in predicting the percentage of CO2 uptakes and heat adsorption. This function that is created by the ANN procedure is then employed as a fitness function in the optimization phase. Following the selection of the population and the optimization operations, a Pareto graph is formed as shown in

Figure 9, The Pareto frontier is achieved by solving the optimization model with the LM method Figure 9. Optimum point of optimization. From the optimization result with the prediction equation by ANN the optimal values for CO2 and heat adsorption were maximum at 35.25% and 33.8% and the

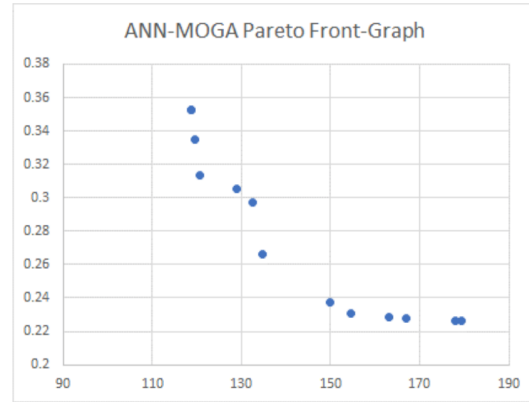


Figure 9 ANN MOGA Optimization minimum is at 23% respectively for both of them.

### 4. Conclusion

Over the last two decades, the development of porous MOFs for CO2 capture and storage (CCS) has accelerated. MOFs have exceptional features such as high surface areas, thermal stability, chemical stability, and easily adjustable and diverse architectures. The chemical characteristics of the adsorbent do not always determine the viability of capturing CO2 in industrial flue gas. Cost, environmental compatibility, safety, parasitic energy loss, heat management, thermodynamic efficiency, humidity stability, robustness, recyclability, and kinetics all have a significant impact on CO2 capture effectiveness. We examined adsorption and built adsorption systems in this review. The first stage in improving CO2 collection is the creation of adsorbents that significantly improve adsorption system performance.

The requirement for porous and recyclable MOFs for CO2 collection and environmental concerns has fueled the development of biomolecular ligand-based MOFs (bioligands). Multiple guest binding, chirality, self-assembling capabilities, and flexible or robust frameworks are among the qualities of the bioligands used to form bio-MOFs that make them excellent for CO2 collection. Several modes of bio ligand binding have been investigated. Because of the availability of amino acids, peptides, nucleobases, saccharides, porphyrins, and proteins in nature, a wide range of bio-MOF structures have been developed. Lewis

bases are found in carboxyl-, nitrogen-, and metal-bearing ligands, which can improve CO<sub>2</sub> adsorption.

Bio-MOFs have a high capacity for CO<sub>2</sub> adsorption applications. Only under post combustion CO<sub>2</sub> capture settings at ambient pressure and temperature has the great selectivity of bio-MOFs been tested. Bio-MOFs have not been thoroughly investigated in precombustion conditions, which include high pressures and temperatures.

More research on the effectiveness of bio-MOFs for pre combustion CO<sub>2</sub> capture is thus required. The influence of adsorption heat on adsorption capacity and selectivity, as well as structural optimization of bio-MOFs, have not been thoroughly investigated.

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The enthalpy values of existing bio-MOFs with excellent adsorption capabilities and selectivity are high. Heat and energy management in industrial CO<sub>2</sub> adsorption systems will be affected.

More research on the use of bio-MOFs for CO<sub>2</sub> capture is required, particularly on the impact of chemisorption on adsorbent characteristics and system parameters that affect energy consumption, cost, and thermodynamic efficiency. We believe that many future studies will concentrate on optimizing bio-MOF adsorption in terms of both energy usage and adsorption efficiency cost. Dynamic tests at various CO<sub>2</sub> concentrations should be carried out in order to produce an optimal CO<sub>2</sub> adsorption system suited for industrial use.

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