# SIIC005

## PROCESS MODELING OF SONOCATALYTIC DEGRADATION OF CAFFEINE USING $CeO_2$ VIA BLACK BOX METHOD

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***Abstract:***
In order to meet human demands, the pharmaceutical industries are increasing over the years. Caffeine ($C_8H_{10}N_4O_2$), representative as one of the pharmaceuticals and personal care products (PPCPs) was considered to be contaminating to humans and other aquatic life which has exerted water pollutions crisis. In this study, the mathematical modeling of sonocatalytic degradation of caffeine using $CeO_2$ was developed via artificial neural networks. The artificial neural network (ANN) was employed for developing the suitable modeling of the $CeO_2$ catalyst in determining the efficiency of sonocatalytic degradation of caffeine using $CeO_2$ (%). The parametric conditions of this study involved initial pH of caffeine, initial concentration of caffeine (g/L), and dosage of $CeO_2$ (g/L). Thus, a three-layered feed-forward back propagation neural network with 12 neurons in the hidden layer was built to give the optimal results on the efficiency of sonocatalytic degradation of caffeine using $CeO_2$. ANN predicted high accuracy in which $R^2$, MSE, and MAE values were 0.996, 0.3109, and 0.07885 respectively. It was also revealed that the ANN model was provided excellent predictive performance by giving the highest value of $R^2$.

***Keywords*:**
Artificial neural network; Modeling; Caffeine; Sonocatalytic degradation; $CeO_2$

***Objectives:***

- To develop a mathematical of sonocatalytic degradation of caffeine using $CeO_2$ via an artificial neural network (ANN).
- To evaluate the model prediction ability by experimental results from previous study.

***Methodology:***

Data generation from a previous study done by Nur Fadzeelah et al. [1]

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Developed ANN model with ratio of training, validation, and testing of the network was designated as 70:15:15

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The MSE, mean absolute error (MAE), and coefficient of determination ($R^2$) were evaluated to predict the performance of ANN.

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Developed another model to test the fact of predictive capabilities of the ANN model with the same 4:12:1 topology but in different range values

***Results:***

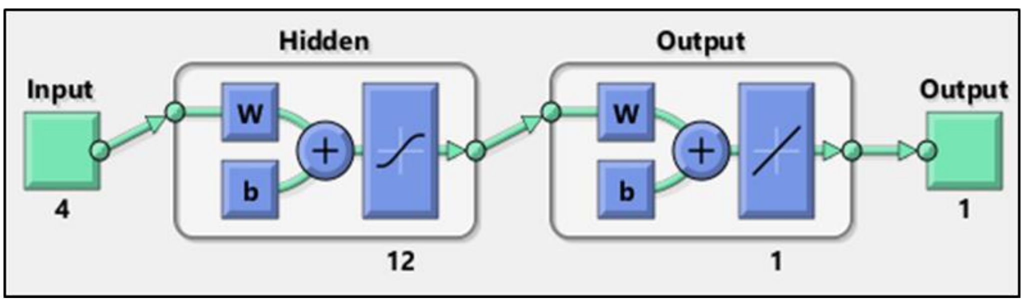
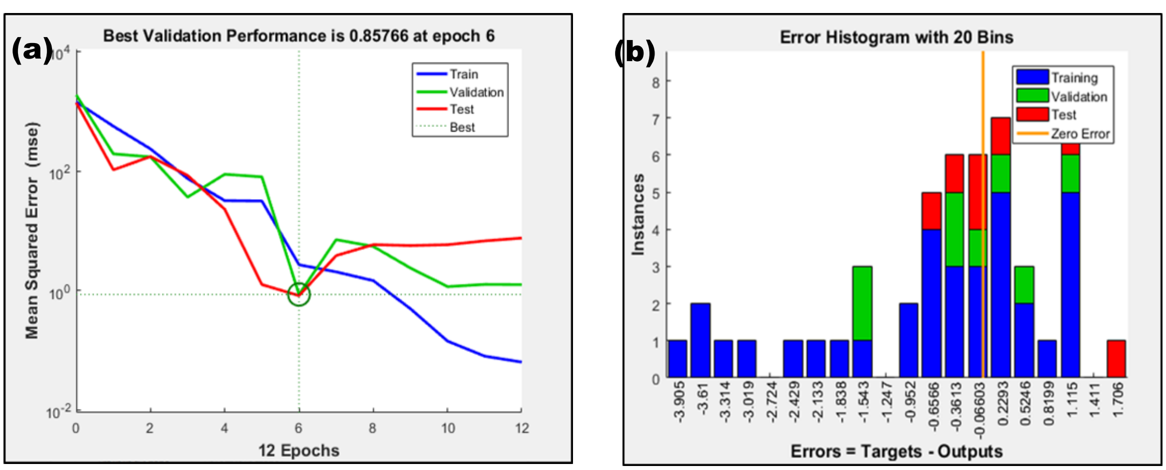



Figure 1 ANN topology design of sonocatalytic degradation efficiency



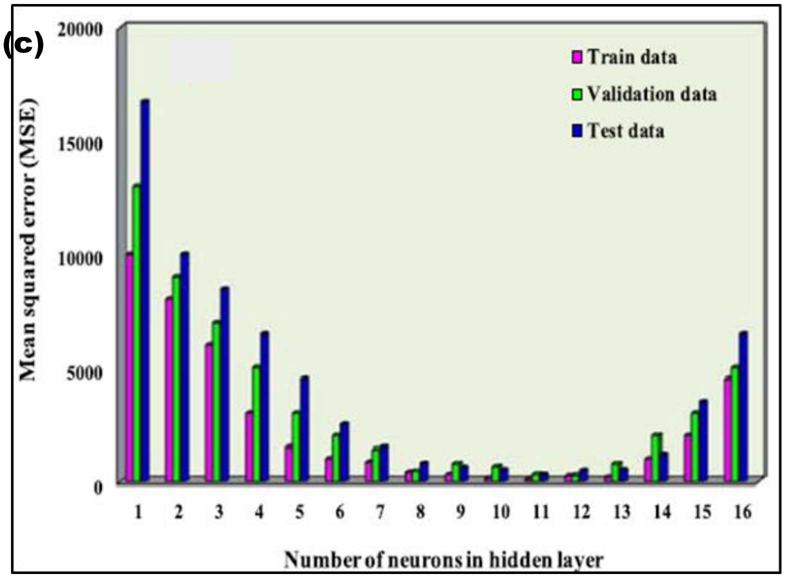



Figure 2 (a) MSE values in the efficiency of sonocatalytic degradation; (b) error histogram of developed ANN model; (c) mean squared errors against the number of neurons in the hidden layer

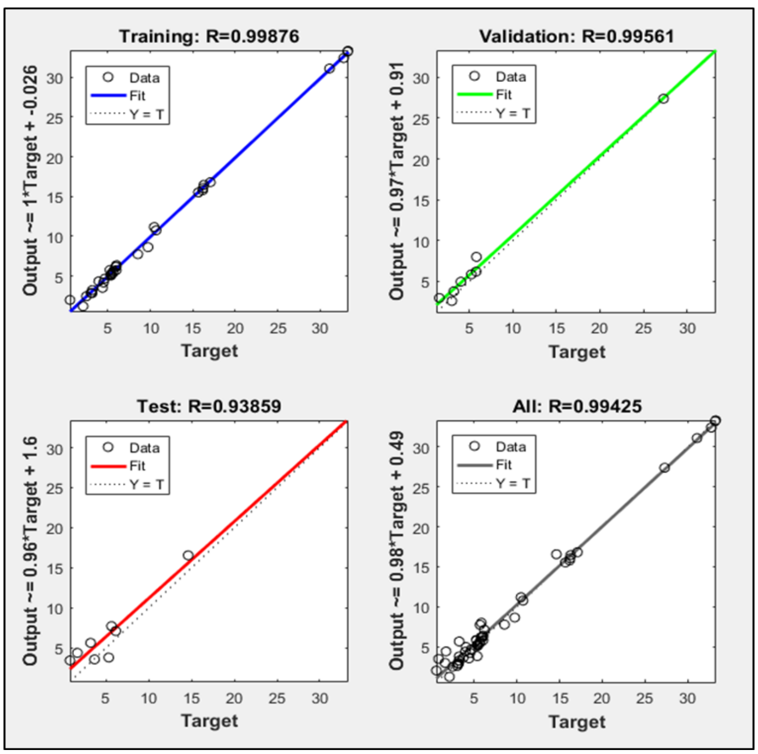



Figure 3 regression plots for training (a); validating (b); test (c); and total data (d)

Table 1 Efficiency of ANN developed model

| Developed Model | $RE_{predicted}$ | $R^2$ | MSE | MAE |
|---|---|---|---|---|
| ANN | ANN with 4:12:1 topology | 0.994 | 0.3109 | 0.07885 |

*$R^2$: Correlation coefficient; MSE: Mean squared error; MAE: Mean absolute error

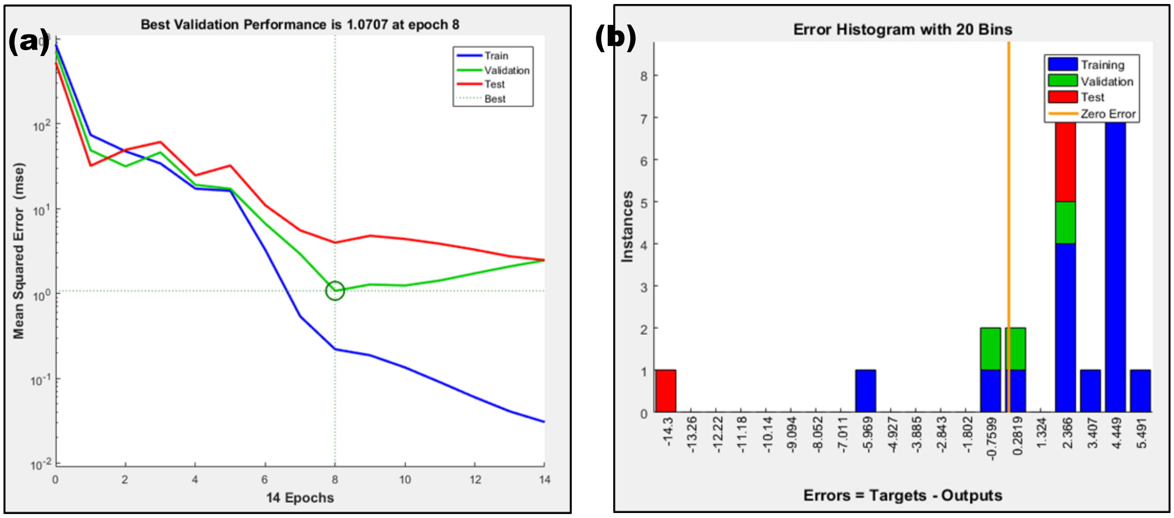



Figure 4 (a) MSE values in the modeling of sonocatalytic degradation efficiency; (b) error histogram of the ANN test model

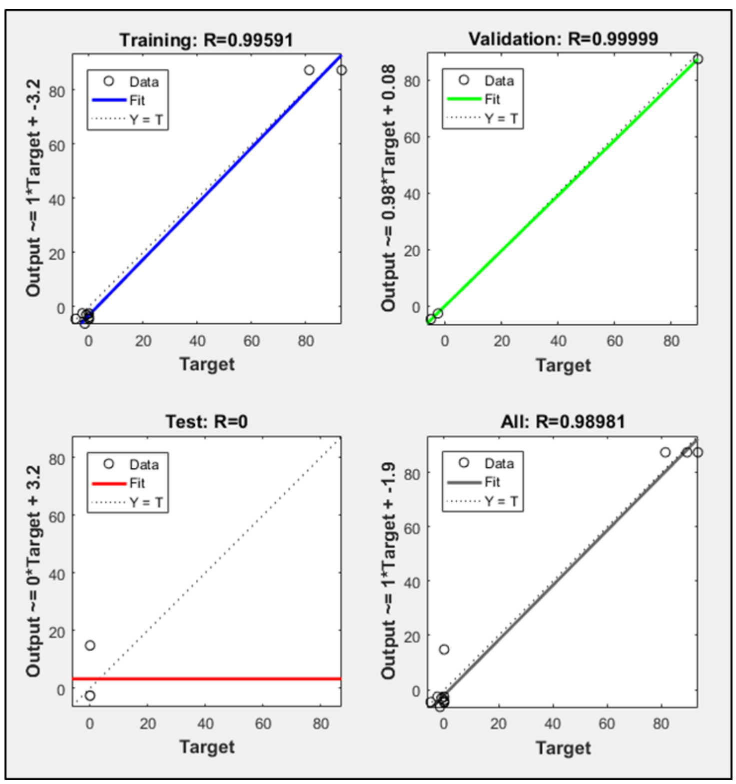



Figure 5 Regression plots of the ANN test model

Table 2 Efficiency of ANN test model

| Developed Model | $RE_{predicted}$ | $R^2$ | MSE | MAE |
|---|---|---|---|---|
| ANN test models | ANN with 4:12:1 topology | 0.989 | 0.0721 | 0.0560 |

*$R^2$: Correlation coefficient; MSE: Mean squared error; MAE: Mean absolute errors

***Conclusion:***

In this research work, the main aim of the present study was to model and predict the efficiency of sonocatalytic degradation of caffeine using $CeO_2$. To achieve this aim, the artificial neural network modeling based upon the black box method was successfully applied to demonstrate the caffeine degradation in an aqueous suspension using commercial $CeO_2$ nanoparticles. The ANN models showed a good agreement between the predicted caffeine removal efficiencies and the experimental results were also achieved ($R^2$ values was 0.994). The whole of this studies give some new knowledge and information about the sonocatalytic degradation mechanism using ANN modeling, which can be valuable to design and model the different industrial parameters. As a final observation, it can be conclude that the ANN model is set up to be able of having a huge ability for the prediction of sonocatalytic degradation of caffeine using $CeO_2$ efficiency at various parametric conditions and the ANN has successfully exposed that the predicated model was fitted perfectly with the experimental data giving the highest value of $R^2$. In addition, this work provides an understanding statistical modeling which could provide exposure for developing an optimized nanomaterial towards the removal of micropollutants accurately.