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Machine Learning-Predictive Modelling of Calcium Removal from Cooling Tower Water Using Amberlite IR120 Resins

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INTRODUCTION & AIM

The global increase in industrialization and quick development resulting from the Industrial Revolution has led to a continuous rise in wastewater output.[1] The methods to remove heavy metals from aqueous solutions are reverse osmosis, ultrafiltration, chemical precipitation, adsorption and ion exchange. The ion exchange process (IEX) effectively reduces heavy metal concentration because it is environmentally friendly, economically viable, selective, and less sludge volume produced.[2] The buildup of scale in cooling systems, especially evaporative cooling systems, is frequently a significant problem because of calcium (Ca) ions in raw or makeup water. As water evaporates, the concentration of these ions increases, leading to the formation of insoluble salts such as ($CaCO_3$). [2]

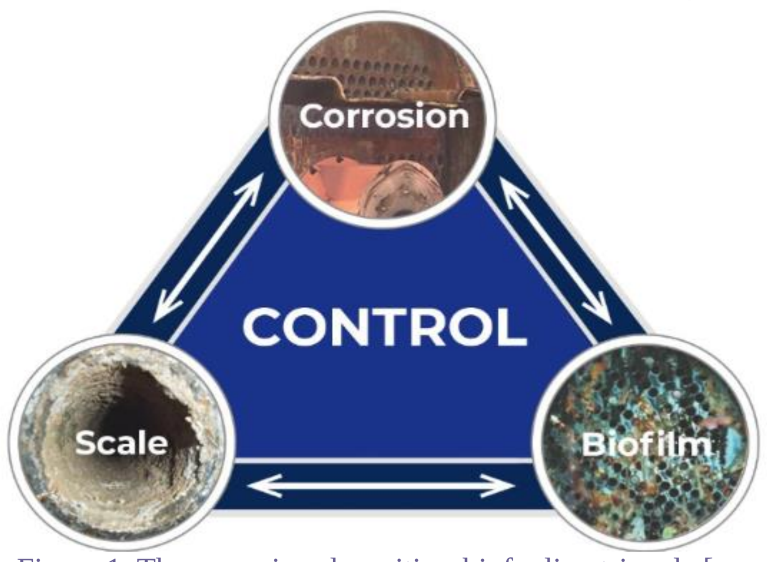

Figure 1. The corrosion-deposition-biofouling triangle [source: ChemTreat]

Figure 1 shows challenges encountered in cooling water treatment. Machine learning provides the best predictive modelling with the highest accuracy, inspired by the brain's autolearning and self-improving capability to solve the study's complicated questions; therefore, it is beneficial for modelling transesterification processes.[3]

The present study investigated the removal of Ca^{2+} from cooling tower water using Amberlite IR120 and predictive machine learning approaches. Response surface methodology (RSM), artificial neural network (ANN), and adaptive neuro-fuzzy inference system (ANFIS) were for predictive modeling of calcium removal.

METHOD

The experiments carried out in this study were conducted using Amberjet 1200. These experiments were carried out by varying the set points conditions of process variables as per experimental design in Table 1, noting the output as removal percentages Ca^{2+}. Column setup was used as shown in Figure 2.

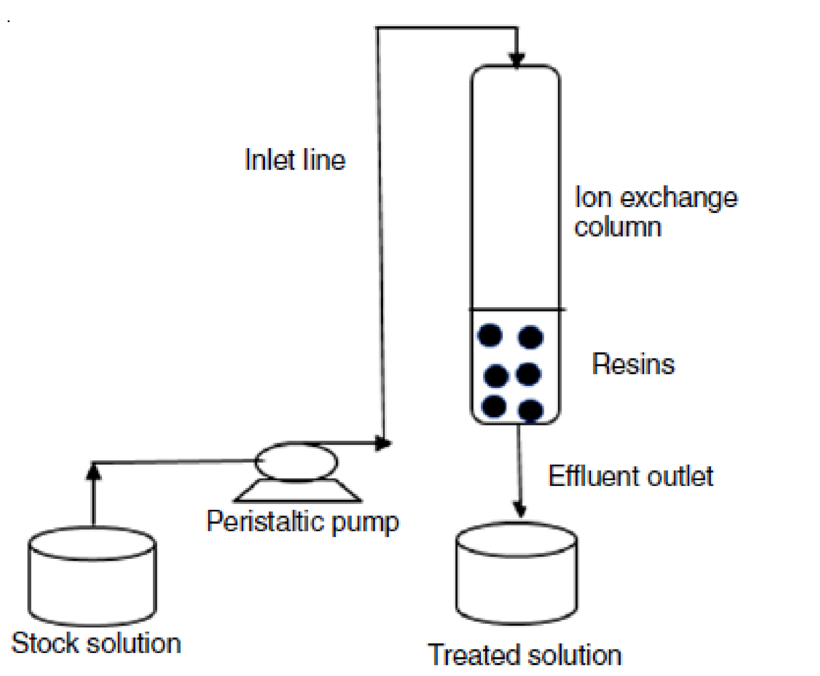

Figure 2. Experimental setup for ion exchange column

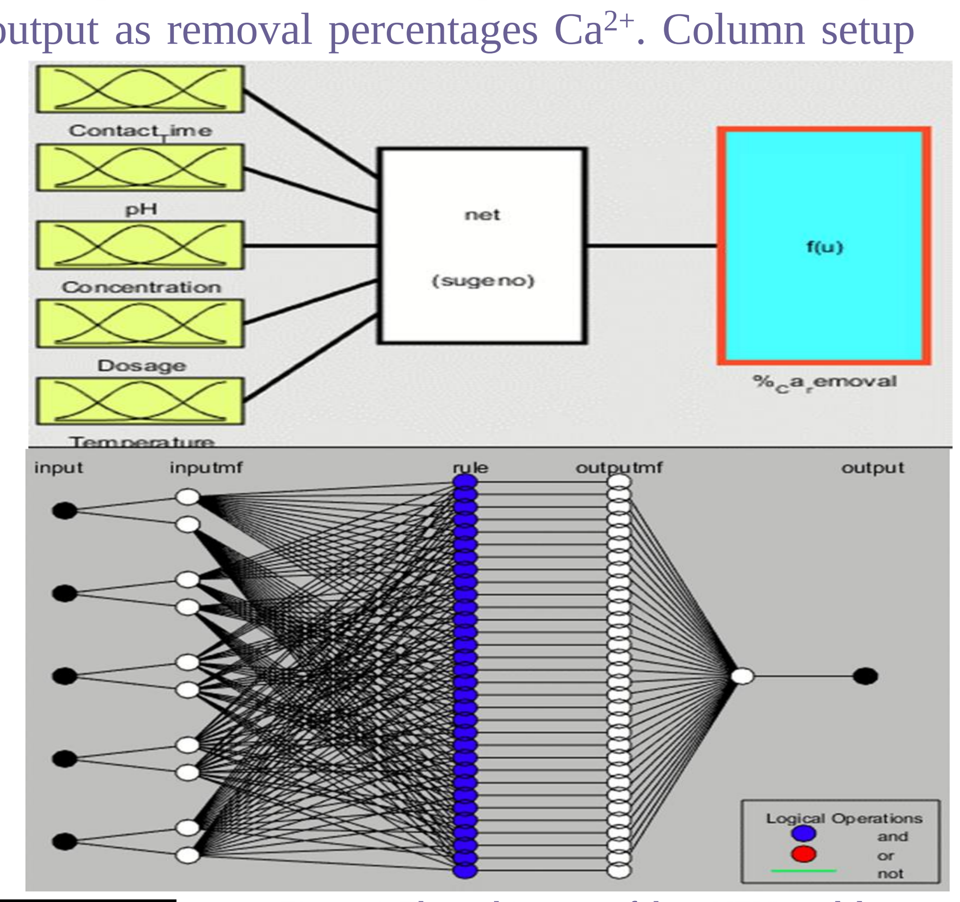

Figure 4. The architecture of the ANFIS model

Table 1 Experimental design

Input	Levels			Output
Variables	-1	0	+1	Ca^{2+} removal (%)
Contact time (min)	30	75	120	
pH	2	4	7	
Concentration (mg/L)	400	600	800	
Dosage (mL)	50	100	150	
Temperature (K)	273	308	343	

$$\text{Removal } (\%) = \frac{C_i - f}{C_i} \times 100 \quad (1)$$

The removal % was calculated using Equation 1, where C_i and C_f are the initial and final concentrations (mg/L), respectively.

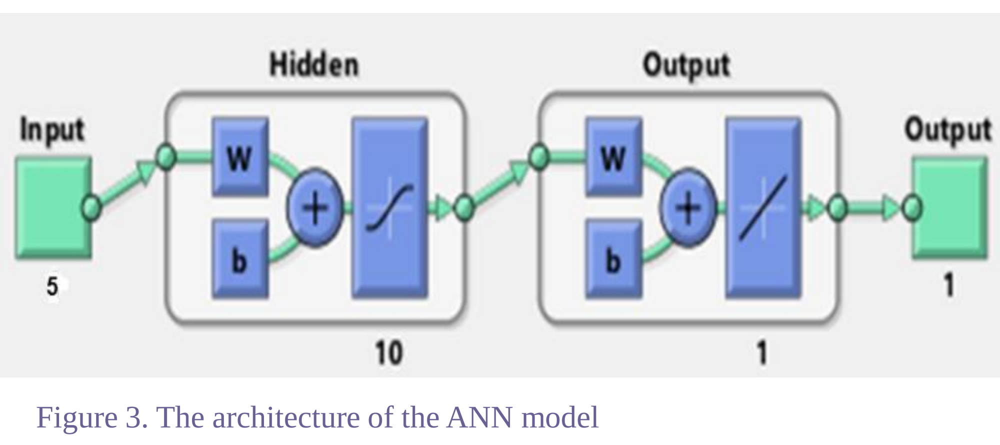

Figure 3. The architecture of the ANN model

5 Four process variables were used and input variables: contact time, pH, Concentration, Dosage and Temperature. RSM was applied in Design Expert 13, and Neural Network Modular and Neuro-fuzzy were built with an NN toolbox using MATLAB 2021. 32 experimental data were randomly divided using the *dividerand* function into 70 % for training and 30% for validation and testing.

The ANFIS was generated using a grid partition and trained using a hybrid method; 80% was used for training, and 20% was used for checking.

RESULTS & DISCUSSION

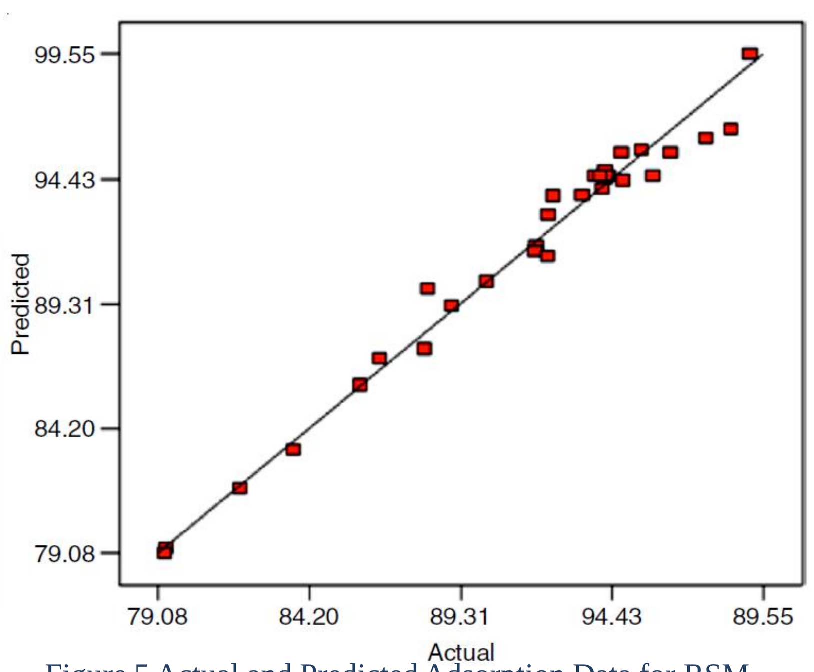

Figure 5 Actual and Predicted Adsorption Data for RSM

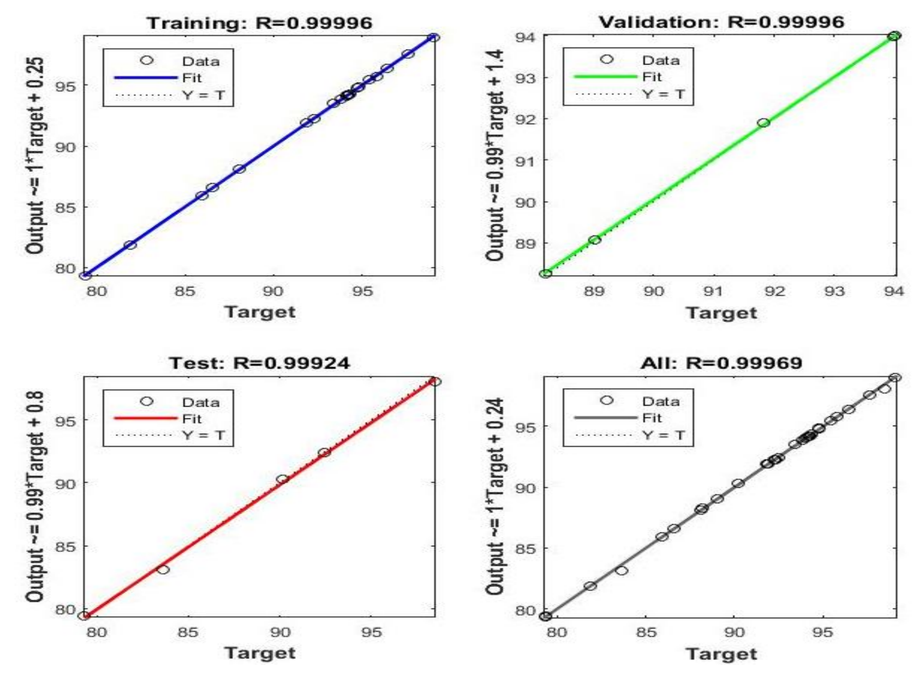

Figure 6: Training, validation, and testing for the ANN Model.

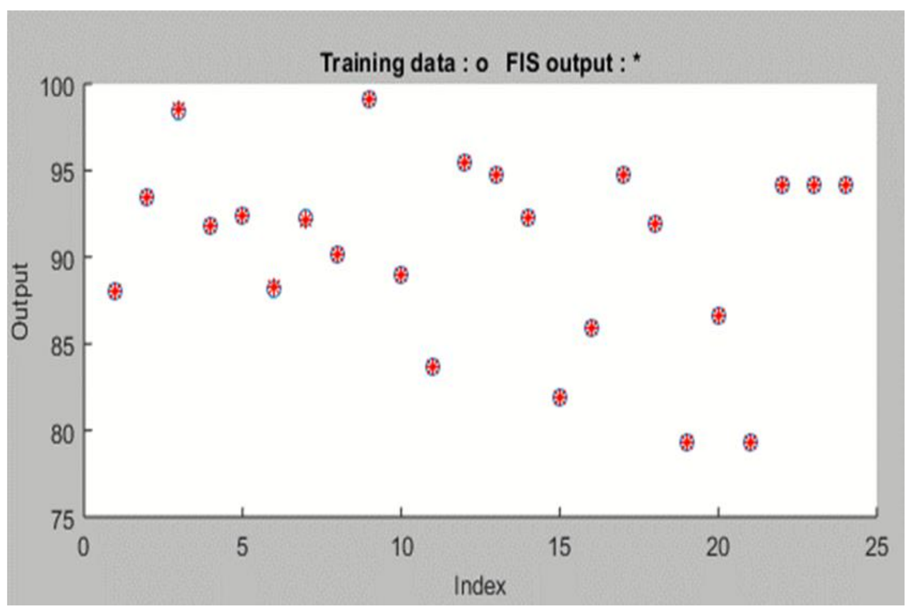

Figure 7 Actual and Predicted Adsorption Data for ANFIS

Figures 5, 6 and 7 show actual and predicted removal % of the 3 models used. All the points are close to the line of experimental, showing the robustness of the model built. This shows that using Amberjet 1200 for calcium removal, high removal efficiency was obtained, and also high predictive model efficiency was achieved

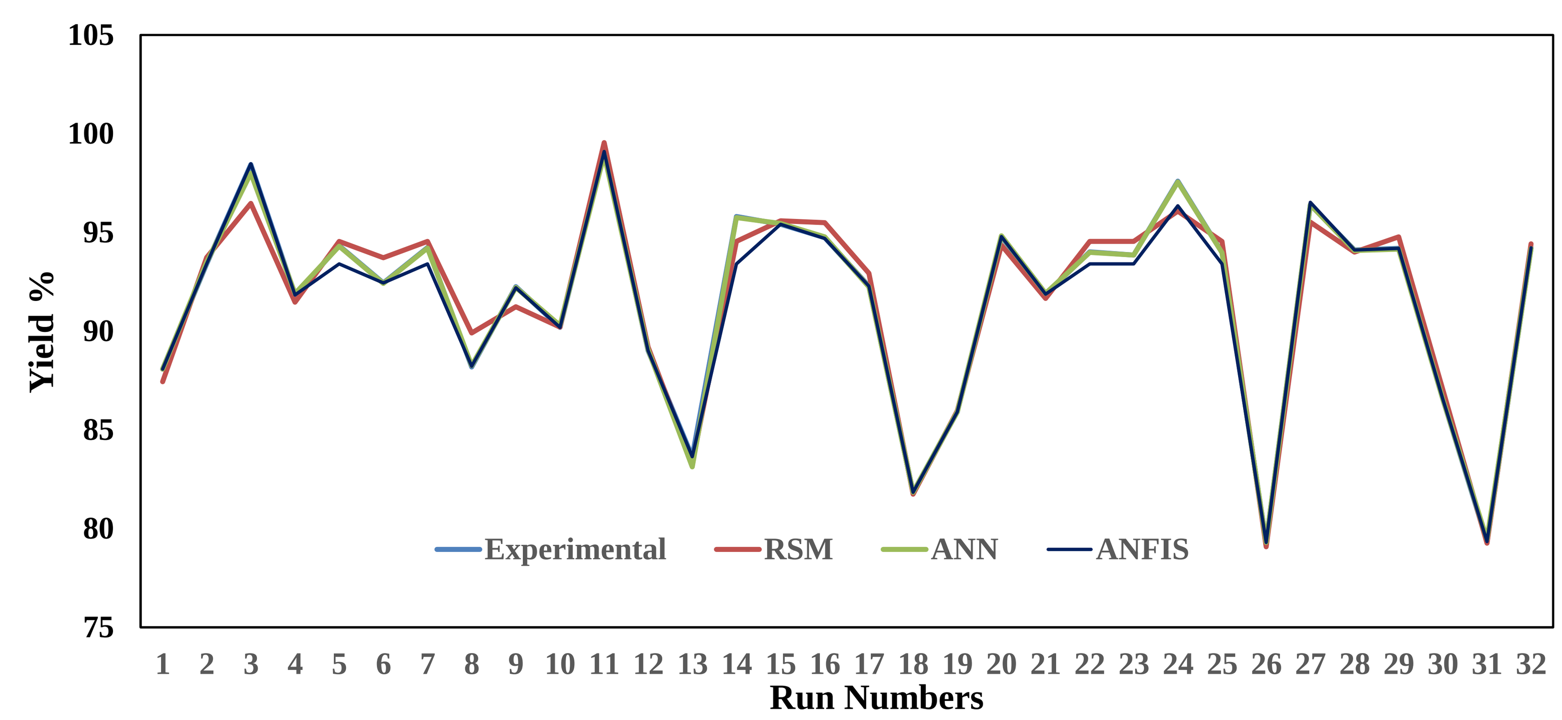

Figure 8 Comparison of experimental, RSM, ANN, and ANFIS removal percentage yield.

Table 2: Error metrics used to evaluate the models

Evaluation metrics	RSM	ANN	ANFIS
R^2	0.9777	0.9994	0.9903
MSE	0.5727	0.017	0.3087
RMSE	0.7568	0.1303	0.5556
MAE	0.5716	0.0677	0.2300
MAPE	0.6135	0.0744	0.2414
ARE	0.0061	0.0007	0.0024
MPSD	11.106	1,3157	4,4689

From the evaluation metrics used to evaluate the effectiveness of the models, All the predictive modelling used are suitable to predict the removal efficiency of Ca^{2+} as there was not much difference as shown in Figure 8 and as shown in Table 2. ANN outperformed with high R^2 and low error metrics.

CONCLUSION

Numerical optimisation yielded an optimal removal percentage of Ca2+ of 99.07% at 89.55 minutes, 4.17, 452.83 mg/L, 132.57 ml and 295.58 K. The developed predictive machine learning model fits the 3 machine learning models with regressions of 0.9777, 0.9994, and 0.9903 for RSM, ANN, and ANFIS, respectively. This study has shown machine learning to be an effective tool for removing Ca2+ from cooling water Amberlite IR120 resins.

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[2] Mbedzi, R.; Rutto, H.; Seodigeng, T.; Sibali, L. Optimization of Ca^{2+} Removal from Cooling Tower Water Using Amberlite IR120 and Amberjet 1200 Resins: A Response Surface Methodology Study. Asian J. Chem. **2023**, 35 (11), 2739–2748.
[3] Xing, Y.; Zheng, Z.; Sun, Y.; Agha Alikhani, M. A Review on Machine Learning Application in Biodiesel Production Studies. Int. J. Chem. Eng. *2021*, 2021, 1–12.