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Applications of Machine Learning in Modelling and Optimization of Breakthrough Curve Analysis: A Focus on Artificial Neural Network and their Comparison

Muhamad Afif Naqiudien Aladin[1], Zykamilia Kamin[1,*], Chiam Chel-Ken[1], Mohd Hardyianto Vai Bahrun[2], Awang Bono[3]

[1] Oil and Gas Engineering Programme, Faculty of Engineering, Universiti Malaysia Sabah, Jalan UMS, 88400, Kota Kinabalu, Sabah, Malaysia
[2] Department of Chemical Engineering, Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bharu, Johor, Malaysia
[3] Faculty of Business Management and Information Technology, Universiti Muhammadiyah Malaysia, Padang Besar 02100, Perlis, Malaysia

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ABSTRACT

Complex processes like adsorption in fixed-bed columns can now be optimized thanks to the application of machine learning (ML) and deep learning (DL) in chemical engineering. One of the most important metrics for assessing adsorption performance in packed bed columns is breakthrough curve analysis. However, predicting breakthrough curve is not an easy task due to high complexity between the adsorbate and desorbent interactions. Different adsorption system requires different ML algorithm types with distinct configurations and hyperparameters. Hence, this article discusses the performance of various artificial neural networks (ANNs) architectures and hyperparameters in predicting breakthrough curves from various published literatures. We also evaluate ANNs configurations, optimization approaches, and performance metrics against traditional techniques and other machine learning algorithms, such as Random Forest, XGBoost, and Support Vector Machines. Our review demonstrates how ANNs may capture nonlinear correlations between breakthrough curve factors and adsorption performances. The comparison results highlight that ANNs enhance prediction accuracy and adaptability, establishing it as an essential instrument for dynamic process simulation and optimization. Unlike previous reviews, this work uniquely consolidates and analyzes trends in ANN configurations and hyperparameter effects across diverse adsorption systems, providing new insights into best practices for data-driven adsorption modelling. The findings encourage a wider use of machine learning in process engineering applications and advance data-driven modelling techniques in adsorption science.

1. Introduction

Machine learning (ML) and deep learning (DL) have transformed data-driven problem solving across scientific and industrial domains. With increasing data availability and computational power, ML models can now identify complex patterns between inputs and outputs, providing predictive and analytical capabilities that were previously challenging [1] ML simulates human learning behavior,

* *Corresponding author.*
E-mail address: zykamilia@ums.edu.my

enabling systems to extract knowledge and improve performance iteratively [2]. Consequently, any improvements made in the field of machine learning would improve computer capabilities and thereby affect technological advancement [3]. Many ML algorithms have been used in recent years to help with challenging tasks in industries due to its ability to capture complex pattern in high dimension datasets [4]. One key application is in adsorption, where breakthrough curve (BTC) analysis measures adsorption performance in fixed-bed systems. Predicting BTCs is challenging due to the intricate interactions between adsorbate and adsorbent. Numerous parameters such as flow rate, concentration, and bed height influence the adsorption process, requiring models capable of capturing nonlinear dependencies. This paper reviews literature on the influence of ANN configurations and hyperparameters on BTC prediction and compares the performance of ANN and other ML models in adsorption studies.

2. Fundamentals of Adsorption and Breakthrough Curve

Adsorption is defined as an increasing concentration of a particular substance at the surface of the interface between two phases. These particular substances transition between phases and then adhering to a surface. It is regarded as a complicated phenomenon that mostly depends on specific adsorbate and the surface chemistry or nature of the adsorbent, as well as the system circumstances between the two phases in a bulk of fluid. This process is preferably being analyzed in a cylinder container called fixed-bed column due to its simple design and relatively inexpensive [5]. In this configuration, a solution feed that contain the compound that is needed to adsorb will be flowed through the fixed-bed column filled with adsorbent. At the end of the column, the concentration of the adsorbate will be measured hence the graph for the breakthrough curve of the current adsorbate can be plotted for further analysis [6]. Depending on the type of the adsorbate and adsorbent interactions, the shape of the graph will be different. Additionally, several variables including bed height, adsorbate concentration, flow rate, particle size, temperature, pH and other factors are assessed in order to evaluate adsorption performance such as breakthrough time, exhaust time, length of mass transfer zone (MTZ) and column maximum capacity. Due to various number of features and response variables to assess the performance of the adsorption phenomena, ML and/or DL have been common options for researchers to predict the breakthrough curve since it can capture the complex pattern between the input features and output parameters without understanding the phenomena. Fig. 1 shows the typical shape of breakthrough curve graph.

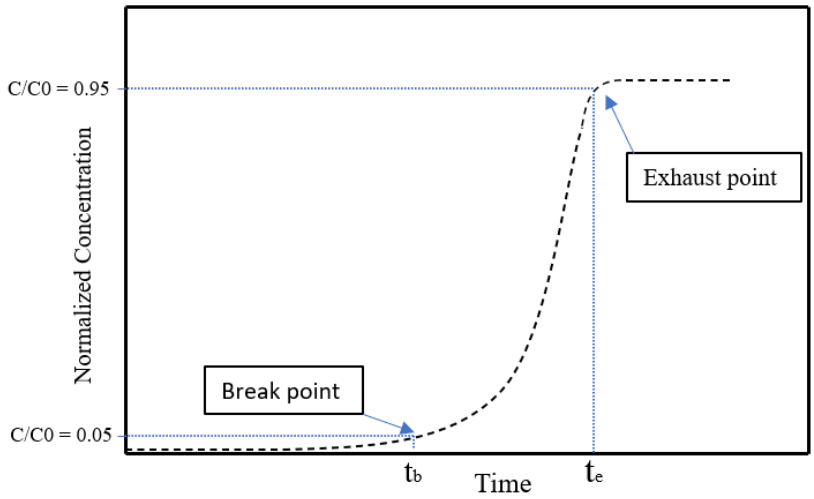

Fig. 1. Illustration of typical breakthrough curve

3. Understanding Artificial Neural Network

Artificial Neural Networks (ANNs) mimic the human brain's processing by using interconnected layers of neurons that learn from data [7]. In supervised learning, ANN learn from large datasets by identifying relationships between input and output variables [8]. Activation functions determine how signals move between layers, while training algorithms such as backpropagation and Levenberg–Marquardt help the network minimize prediction errors and improve accuracy [9].

Before training, ANNs require setting hyperparameters like the number of layers, neurons, learning rate, and activation functions [10]. Selecting these properly affects model performance and helps avoid overfitting or underfitting [11]. Automated optimization methods are being developed to streamline hyperparameter tuning [12]. ANNs can model nonlinear, complex systems that traditional mathematical models cannot easily capture [13]. They are flexible, adaptive, and capable of handling noisy or incomplete data [14]. Their strengths include real-time learning, fault tolerance, and the ability to generalize patterns across different datasets [15].

4. Applications of Artificial Neural Network in Breakthrough Curve Study

ANNs have become an important tool in predicting and optimizing adsorption processes due to their ability to model nonlinear relationships. Traditional models often fail to capture the complexity of adsorption dynamics, while ANNs can learn these patterns from experimental or simulated data. Several studies confirm ANN's superior predictive ability. Atta [16] achieved R^2 = 0.999 for tetracycline adsorption on rice husk. Schio *et al*., [17] reported better accuracy of ANN than response surface methodology (RSM) for FD&C Red 40 dye adsorption. Das and Mishra [18] found that optimizing hidden neurons improved iron ion adsorption prediction. Gupta and Kumar [19] demonstrated higher R^2 (0.99907) for xylene vapor adsorption using ANN compared to RSM.

Further applications include variable ranking and sensitivity analysis. Dalhat *et al*., [20] found concentration and flow rate to be dominant factors in phenol and ortho-cresol adsorption. Yusuf *et al*., [21] applied ANN to copper and manganese adsorption and confirmed its ability to generalize across multi-variable systems. Chittoo and Sutherland [22] showed that ANN predicted full BTCs better than ANFIS for phosphate adsorption.

Collectively, these studies highlight that ANNs consistently outperform traditional statistical and mechanistic models in modelling adsorption processes due to their ability to capture nonlinear, multidimensional relationships without prior assumptions about system behaviour. Most successful models used feed-forward backpropagation networks with nonlinear activation functions (such as sigmoid, hyperbolic tangent, or logsig) in the hidden layers and linear functions in the output layer, which are well-suited for regression-based prediction tasks like breakthrough curve fitting. The use of training algorithms such as Levenberg–Marquardt backpropagation further improved convergence speed and model accuracy. Moreover, appropriate dataset partitioning—typically 70% for training, 15% for validation, and 15% for testing—was found to enhance generalization and prevent overfitting.

In summary, the reviewed literature establishes ANN as a powerful, reliable, and adaptable tool for adsorption modelling and breakthrough curve prediction. It not only delivers highly accurate performance metrics (often with R^2 values exceeding 0.99) but also provides flexibility in incorporating multiple variables, performing sensitivity analyses, and guiding process optimization. The findings indicate a growing trend toward using hybrid or optimized ANN models combined with other algorithms such as response surface methodology, adaptive neuro-fuzzy systems, and evolutionary optimization techniques. This progression points to a future where ANN-based models

will play a central role in digitalizing adsorption science, enabling faster process design, real-time simulation, and intelligent optimization in chemical and environmental engineering applications.

5. Discussions on the Trends and Insights on the Configurations, Hyperparameters, and Their Implications in ANN Applications for Adsorption Breakthrough Curve

Datasets Variations. Analysis of ANN configurations reveals notable trends as presented in Table 1. The range in dataset sizes, from as few as 10 data points to over 1,200, is among the most obvious findings. While there is no true analytical method on how many datasets generations are desirable for each of the adsorption system, it is desirable to train the datasets by a little and increase its number until the model achieves adequate accuracy. Additionally, despite this big variance in the dataset's requirement, most researches use a training, validation, and testing split of roughly 70:15:15 or 70:10:20, which is consistent with supervised learning best practices to guarantee strong generalization and efficient model training. However, some researches either leave the data partitioning unclear or did not provide the datasets split (e.g., Sutherland, 2020). These omissions restrict the interpretability of stated model performance and hinder reproducibility.

ANN Architectures. Most research use relatively simple to moderately complicated architecture, usually consisting of one to three hidden layers, when it comes to ANN design. Neuron counts vary greatly between layers, with common configurations being 1-1-1-1, 3-10-1, 5-5-1, and 4-30-1. It is clear that when the model is properly suited to the problem and dataset size, ideal predictive performance can be attained even with moderate architectural complexity. For example, using only 96 data points and a 3-6-6-6-1 structure, Gupta and Kumar (2021) found an R^2 value of 0.99007, suggesting that careful model design and data handling are just as important for performance as network depth.

Activation Functions in Hidden and Output Layers. The selection of activation functions also follows standard ANN modelling approaches. The sigmoid, hyperbolic tangent (tanh), and their variations (such as logsig) are the most used hidden layer activation functions because of their ability to simulate the nonlinear relationships that are typical for adsorption processes. The output layer uses a linear activation function in almost every system, which is suitable for regression applications like breakthrough curve prediction. The suitability of ANN for producing continuous value predictions in this case is further supported by the regular use of linear output activations. While most of the ANNs rely on the common activation functions (sigmoid, linear), it is recommended to try other types as well since they might give higher accuracy with faster converge time and simpler ANN architectures.

Performance Metrics of ANNs. The ability of ANNs to provide incredibly precise representations of breakthrough behaviour is demonstrated by the model's performance as determined by statistical metrics like the coefficient of determination (R^2), mean squared error (MSE), and root mean squared error (RMSE). R^2 values above 0.99, which indicate excellent model fit, are reported in most numbers of study. As evidence of the reliability of ANN models when set up correctly, Atta [16] and Schio *et al*., [17], exhibit high R^2 values with corresponding low error terms. Some models, however, perform comparatively worse. For example, Chittoo and Sutherland's [22] model produced an R^2 of 1.0 but an RMSE of 1.5628 and an MSE of 2.4423. This discrepancy could be the result of inconsistent feature selection and data preprocessing, overfitting, or a less-than-ideal design. These results highlight how important architecture tuning and dataset quality are to producing precise and useful predictions. It is also worth noting that when evaluating the performance of neural network model, do not rely only on one metrics. It is better to use more than one metrics such as R^2 combines with MSE and RMSE to confirm that the model is not overfitting (memorize the training datasets) or inconsistent.

In summary, ANNs remain effective for BTC prediction, even with limited data, provided architectures and hyperparameters are properly chosen. The trend is shifting toward hybrid ANN models and automated optimization using genetic or Bayesian algorithms to enhance generalization. Future research should prioritize multicomponent systems, larger datasets, and digital twin integration to enable real-time simulation and optimization.

6. Comparison between Different ML Algorithms on Adsorption Study

In recent years, a wide range of machine learning (ML) algorithms—such as Decision Trees, Random Forests, XGBoost, Support Vector Machines (SVM), and Artificial Neural Networks (ANNs)—have been applied to adsorption studies. Each algorithm offers distinct advantages, making the selection of the most suitable model dependent on the nature of the dataset and the prediction goals. Researchers have compared these algorithms to determine which performs best in modelling breakthrough curves and optimizing adsorption processes.

Halalsheh *et al*., [23] explored boosted regression tree techniques, including AdaBoost, Gradient Boosting, XGBoost, LightGBM, and CatBoost, for modelling selenite adsorption on modified zeolite. Among them, CatBoost showed the highest accuracy, with the best agreement between predicted and experimental breakthrough data [23]. Kwon *et al*., [24] tested several ML algorithms which are Decision Tree, Random Forest, XGBoost, Ridge, and SVM variants to predict the location and mass of river contaminant spills using breakthrough curve data. Their findings revealed that Random Forest provided the most accurate and cost-effective results, while XGBoost demonstrated stronger field applicability [24].

In another study, Zhang *et al*., [25] applied the Least Squares Support Vector Machine (LSSVM) to predict gas-side mass transfer coefficients in CO_2 absorption systems. The LSSVM model with a radial basis function (RBF) kernel achieved better prediction accuracy than traditional ANN and regression models, proving its effectiveness for complex gas absorption problems [25]. Similarly, Aftab *et al*., [26] compared multilinear regression (MLR), Support Vector Regression (SVR), and ANN for predicting heavy metal adsorption. Both ANN and SVR models showed excellent predictive accuracy ($R^2 > 0.99$), but SVR slightly outperformed ANN in terms of lower error values and better generalization on test data [26].

Lastly, Yao *et al*., [27] compared Random Forest and Deep Neural Network (DNN) models to predict the purity of products in simulated moving bed (SMB) separation processes. Both models achieved very low prediction errors, but the DNN model demonstrated higher optimization ability, successfully identifying improved process conditions beyond the training data range [27].

Overall, these studies indicate that while ANNs and SVR remain top performers for adsorption modelling, tree-based ensemble methods like Random Forest and XGBoost are equally powerful for specific applications due to their robustness and interpretability. The choice of algorithm ultimately depends on the problem complexity, data volume, and need for optimization. Importantly, deep learning models such as DNNs are showing growing potential, offering faster simulation speeds and the ability to generalize to new operating conditions, making them highly valuable for future process modelling and real-time optimization in adsorption systems.

7. Conclusion

The use of machine learning in modelling and optimizing the adsorptive separation process is covered. A compilations recent published papers examined how ANN can perform better in a variety of adsorption systems than conventional statistical and mechanistic models. To achieve high

accuracy in predicting results output, ANN models have successfully integrated parameters including pH, bed height, influent flow rate, and initial concentration. ANNs have demonstrated better prediction outcomes than other methods in numerous instances. The other alternative ML models covered in this work include support vector machines, XGBoost, random forests, and decision trees. ANN provides far more precise and reliable predictions for the design and optimization of adsorption separative processes, even though these models have some advantages. Future research might be implementing ML hybrid model could lead to a more effective and economical method as much more different ML algorithms will be created in the future.

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Table 1
Summary of optimized ANN configurations from literatures

Name of Authors	Number of datasets (training, validation, test)	ANN configuration	Hidden layer activation function	Output layer activation functions	Model Performance metrics
Atta (2024)	Not specified (70,15,15%)	1-1-1-1	Sigmoid	Linear	R^2(0.999)
Schio, Salau, Mallmann and Dotto (2021)	252 (70,15,15%)	3-10-1	Hyperbolic tangent sigmoid	Linear	R^2(0.99) SSE(0.0459) MSE(0.000186)
Das and Mishra (2021)	185 (70,15,15%)	1-13-3 1-10-3 1-7-3	Not specified	Not specified	R^2(0.99) MSE(0.000209)
Gupta and Kumar (2021)	96 (79.12,10.42.10.42%)	3-6-6-6-1	Sigmoidal	Linear	R^2(0.99907)
Dalhat, Mu'Azu, Essa (2021)	100 (70,15,15%)	5-5-1	Sigmoidal	Linear	R^2(0.988) RMSE(0.0472)
Yusuf, Song, Li (2020)	1000 (not specified)	4-10-1	Tanh	Tanh	R^2(0.998)
Chittoo and Sutherland (2020)	562 (70,no validation,30%)	3-13-2	Tansig	Tansig	R^2(1.0) RSME(1.5628) MSE(2.4423)