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Inovações e Soluções Sustentáveis em Engenharia Ambiental

Applications of artificial neural networks in CO_2 capture: mitigating climate change through adsorption processes

Aplicações de redes neurais artificiais na captura de CO_2: mitigação da mudança climática por processos de adsorção

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ABSTRACT

Since the Industrial Revolution, atmospheric CO_2 levels have increased from 280 ppm to 420 ppm by 2022, raising concerns within the scientific community about climate change. Carbon capture through gas adsorption on solid surfaces has emerged as a viable technique to address this issue. This study employed artificial neural networks (ANN) to predict CO_2 uptake on activated carbon under various experimental conditions, using data such as pressure, temperature, adsorbent surface area, and uptake of CO_2 and CH_4. The network was trained, validated, and tested using the Levenberg-Marquardt algorithm in Matlab©, exploring architectures with 10, 15, and 20 neurons. The best performance was achieved with the 20-neuron architecture, yielding an MSE of 3.80×10^{-3} and R^2 values of 0.98347, 0.98328, and 0.97365 for training, validation, and testing, respectively. Additionally, the Garson method was utilized to assess the importance of the input variables, revealing that the most influential variables were surface area at 50.06%, CO_2 molar fraction at 13.92%, and methane molar fraction at 13.89%. These results demonstrate the effectiveness of the ANN model in predicting CO_2 adsorption, highlighting the potential of combining experimental methods with machine learning for the efficient study of greenhouse gas capture while reducing the costs and time associated with laboratory experiments.

Keywords: Activated carbon; Atmosphere; Machine learning

RESUMO

Desde a Revolução Industrial, os níveis de CO_2 atmosférico aumentaram de 280 ppm para 420 ppm em 2022, levantando preocupações na comunidade científica sobre as mudanças climáticas. A captura de carbono por meio da adsorção em superfícies sólidas emergiu como uma técnica viável para enfrentar esse problema. Este estudo utilizou redes neurais artificiais (RNA) para prever a adsorção de CO_2 em

carvão ativado sob diversas condições experimentais, utilizando dados como pressão, temperatura, área superficial do adsorvente e a adsorção de CO_2 e CH_4. A rede foi treinada, validada e testada usando o algoritmo Levenberg-Marquardt no Matlab©, explorando arquiteturas com 10, 15 e 20 neurônios. O melhor desempenho foi obtido com a arquitetura de 20 neurônios, apresentando um MSE de $3{,}80 \times 10^{-3}$ e valores de R^2 de 0,98347, 0,98328, e 0,97365 para treinamento, validação e testes, respectivamente. Além disso, o método de Garson foi utilizado para avaliar a importância das variáveis de entrada, revelando que as variáveis mais influentes foram a área superficial com 50,06%, a fração molar de CO_2 com 13,92% e a fração molar de metano com 13,89%. Esses resultados demonstram a eficácia do modelo de RNA na predição da adsorção de CO_2, destacando o potencial da combinação de métodos experimentais com aprendizado de máquina para o estudo eficiente da captura de gases de efeito estufa enquanto reduz custos e tempo despendidos para estudos em laboratório.

Palavras-chave: Atmosfera; Carvão ativado; Inteligência artificial

1 INTRODUCTION

Following the Industrial Revolution in 1800, atmospheric CO_2 concentrations were around 280 parts per million (ppm). Researchers have determined that the accumulation of greenhouse gases has led to a rise in global temperatures of up to 1.5 °C since 1850. By 2016, CO_2 levels had risen to 400 ppm, causing significant concern within the scientific community (Dayton, 2016). Predictions suggest that a 2 °C increase in global temperatures could occur once CO_2 concentrations reach 450 ppm. By 2022, the National Oceanic and Atmospheric Administration (NOAA) reported a peak CO_2 concentration of 421 ppm (National Oceanic and Atmospheric Administration, 2022).

The concentration of CO_2 in the atmosphere has been increasing over the years due to emissions exceeding the planet's natural sinks' capacity to remove the gas (Lindsey, 2023). Climate change can indirectly cause adverse effects on public health, including alterations in air pollution, the spread of diseases, food insecurity, population displacement, and mental health issues. The potential impact of climate change may reverse the health benefits gained through economic development (Watts et al., 2015).

As the increase in CO_2 emissions is seen as the leading cause of climate change, carbon capture technologies emerge as an important alternative to help address this problem. Technological advancement is necessary to enable the use of renewable

energy sources without carbon dioxide emissions and to facilitate the economic transition. Short-term measures and strategies to reduce human CO_2 emissions, such as carbon capture, are being adopted (Simon, 2013). In this context, capturing pollutants at the source is an essential climate action to prevent CO_2 from reaching the atmosphere. This approach is based on the idea that human emissions can be controlled. However, for this strategy to work, it is essential to consider the urgency of capturing emissions at the source, the possibility of "buying time" for the economic transition, and the fate of the carbon dioxide after its capture or removal from the atmosphere (Ozin and Ghoussoub, 2020).

Some industrial streams may contain fewer pollutants than atmospheric emissions from power stations, making them better suited for CO_2 capture. Therefore, industrial areas are more suitable for the carbon dioxide capture process, such as fermentation industries that produce CO_2 and water or ethanol vapor; cement manufacturing, which contains solid particles that must be separated before the gas capture process; steel and iron industries; and petrochemical plants (Aresta and Dibenedetto, 2021; Rajabloo et al., 2023; United States Environmental Protection Agency, 2023). Gas capture by adsorption for post-combustion gases is a promising technology for large-scale stationary sources and industrial plants (Raganati, Miccio and Ammendola, 2021).

Efforts have been made to apply computational techniques in industry and academia due to the high cost and time demands required for experiments related to adsorption. Given these challenges and the difficulty of using traditional computational methods to solve engineering problems, more straightforward and more versatile methods have begun to be studied (Ghaemi, Dehnavi and Khoshraftar, 2023).

Artificial neural networks (ANN) are machine learning techniques that resemble the learning mechanism in biological organisms. The human nervous system contains neurons connected by axons and dendrites, with their connection regions known as synapses (Kim, 2017).

Synaptic strengths change due to external stimuli, and this process is responsible for learning in living organisms. This biological mechanism is simulated by artificial neural networks, which contain computational units known as neurons connected through weights that function similarly to synaptic strengths. Thus, each input data in a neuron is assigned a weight that affects the computational function of that unit, allowing the network to learn by adjusting the weights that connect the neurons. In this way, an artificial neural network aims to learn a function that relates one or more input data to one or more outputs (Aggarwal, 2023).

The ability of ANNs to model complex and nonlinear relationships between input and output variables is valuable in adsorption processes for treating industrial atmospheric emissions. These processes can be highly nonlinear and dependent on multiple factors. Additionally, ANNs can adapt to changes in system conditions over time, provided they are trained with updated data. This adaptability is crucial in gaseous emission systems, where conditions can fluctuate due to daily variations, changes in the composition of the fuel used in industrial processes, and weather conditions, among other factors. ANNs can generalize from training data to predict unobserved data, making them effective even when training data is limited or does not cover all possible conditions. Unlike equation-based models, ANNs do not require equations to describe the system and can be adjusted for systems of varying sizes and complexities (Petroli et al., 2024).

Artificial neural networks offer several advantages, such as a reduced need for statistical training, the ability to detect nonlinear relationships between dependent and independent variables, and the ability to identify potential interactions between predicted variables (Tu, 1996). However, ANNs also have some drawbacks, including the occurrence of overfitting, a lack of information about the physical properties of the fluid (e.g., estimation of properties and physical variables), and their “black box” behavior—the opaque and complex nature of ANNs that makes it challenging to understand their internal processing and how predictions are generated (Nighojkar et al., 2023).

This study collected experimental data on CO_2 adsorption capacity for both pure CO_2 adsorption and CO_2 adsorption in a CO_2/CH_4 mixture to evaluate the prediction accuracy of the artificial neural network for CO_2 adsorption capacity on commercial activated carbon in single and multicomponent systems. This analysis contributes to applying CO_2 capture technology in industrial plants and developing new climate policies related to carbon emission reduction. This allows for the study of the amount of carbon that can be removed from stationary sources, helping to mitigate global temperature increases and enabling the achievement of the targets set by the Paris Agreement.

This article explores the prediction of gas adsorption using artificial neural networks, detailing each stage of the study in specific sections. The first section discusses the fundamental concepts of ANNs and their application in modeling adsorption processes. Next, the methodology section describes the procedures for experimental data collection and network training. Then the results are analyzed, focusing on the ANN's performance in predicting CO_2 adsorption capacity for mono and multicomponent systems. Finally, the assigned weights and the relative importance of input variables are presented, followed by a discussion on the impact of parameters on the adsorption process.

2 MATERIALS AND METHODS

2.1 Data preparation and analysis

To evaluate the ability of the ANN to predict gas adsorption, experimental data were collected, including the adsorption capacity of activated carbon, operating pressure and temperature, the surface area of the adsorbent used, and the molar fractions of CO_2 and CH_4. To achieve this goal, references from 1995 to 2022 were reviewed using CAPES, Science Direct, and Google Scholar, focusing on keywords related to CO_2 adsorption on activated carbon and neural networks. Data were collected from

tabular results in articles, and for articles with only graphical data, WebPlotDigitizer was used to extract data points for use in Microsoft Excel.

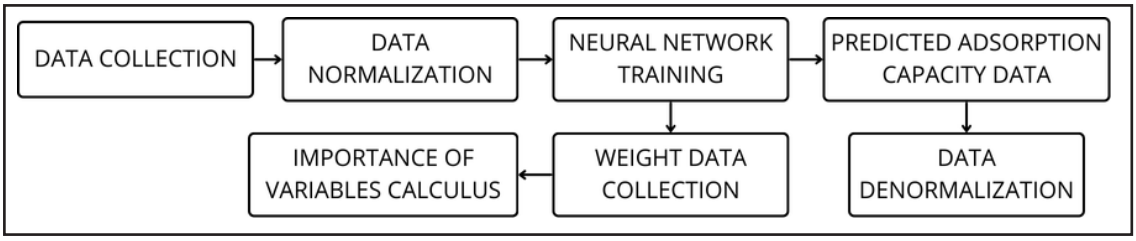
After collecting the experimental data, statistical analysis showed that the data had a normal distribution, which provides a basis for classical statistical inference. Subsequently, due to the different scales of the experimental data, it was normalized in the interval [-1;1] using the min-max method. This choice was made considering the selection of the hyperbolic tangent as the activation function for training the artificial neural network, as this function processes input values and generates outputs within the same specified range. With the data adequately normalized, the ANN was trained using Matlab 2023a through the Neural Net Fitting app.

Min-max normalization was selected over other methods (such as z-score normalization) due to its ability to preserve zero values in sparse data and handle cases when there is a need to map the values to a specific range. This approach ensures that all features contribute equally to the model and prevents features with larger scales from dominating the learning process.

We employed a linear activation function for the output layer to allow the network to produce a wider range of output values, which is often beneficial for regression tasks.

After training the network, the weights of the artificial neural network used during the testing phase were collected to calculate the importance of the variables in the prediction process. Additionally, after obtaining the normalized prediction data, it was necessary to denormalize the data to analyze experimental and predicted values. The methodology is represented in Figure 1 for better understanding.

Figure 1 – Flowchart of the methodology applied



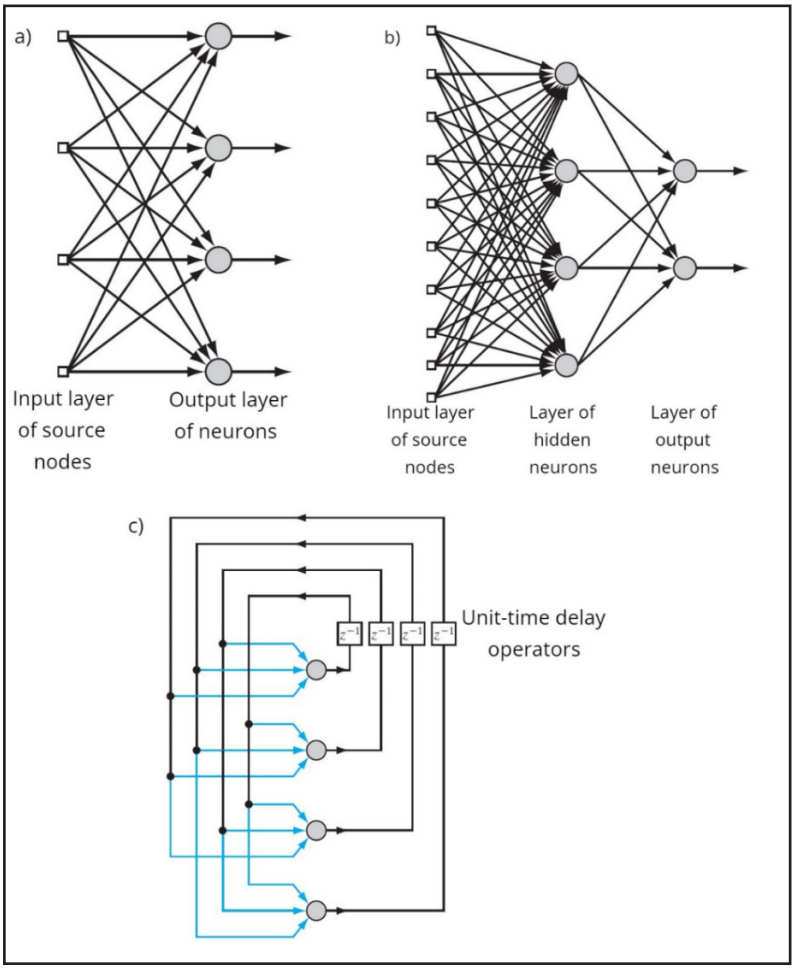
Source: Authors (2024)

2.2 Artificial neural network architecture

The most used structures for architecture are single-layer networks, multi-layer networks, and recurrent networks. In a single-layer network (Figure 2a), an input layer of source nodes is projected onto an output layer of neurons, forming a feedforward network. The network is called feedforward due to the successive feeding of layers from input to output nodes (Figure 2b). Thus, all nodes in one layer are assumed to be connected to those in the subsequent layer. On the other hand, recurrent networks differ from feedforward networks due to at least one feedback loop (Figure 2c). Feedback influences the network's learning capability and overall performance (Aggarwal, 2023; Haykin, 2007).

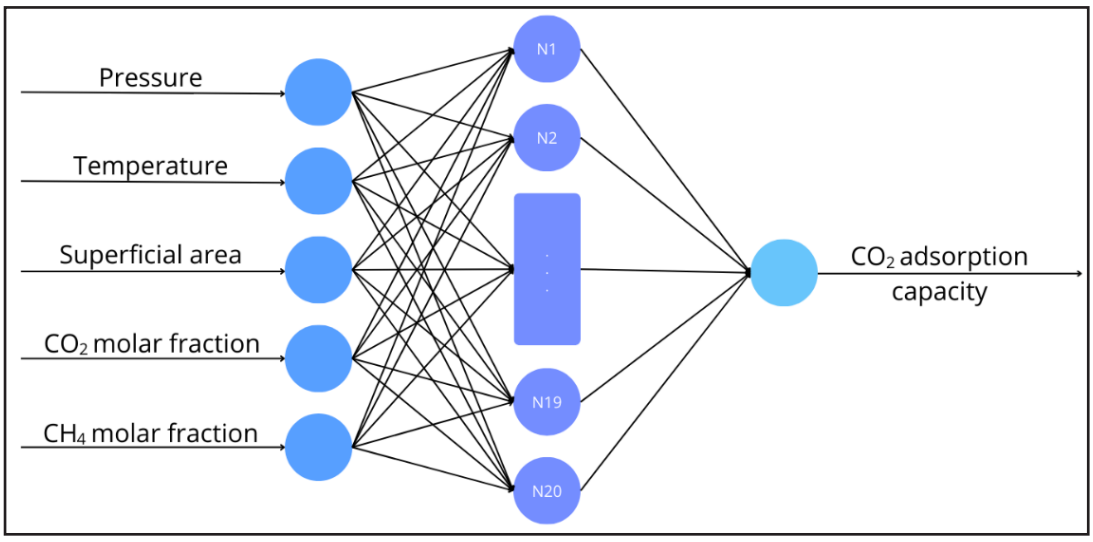
A feed-forward neural network with multiple layers and supervised learning was utilized for prediction. The Levenberg-Marquardt method was employed for network optimization due to its rapid convergence in locating a local minimum of a function. An illustration of the input and output parameters applied to the artificial neural network is presented in Figure 3.

Figure 2 – ANN architecture: a) single-layer networks; b) multi-layer networks; c) recurrent networks



Source: Haykin (2007)

Figure 3 – Representation of the ANN architecture used



Source: Authors (2024)

For the training of the network, a dataset of 2.408 samples was used, divided into 70% for training, 15% for validation, and 15% for testing. The network was trained with three different architectures, each consisting of a single hidden layer containing 10, 15, and 20 neurons. The number of neurons in the hidden layer was determined based on the number of neurons in the input layer. Specifically, since the input layer comprises five neurons, five additional neurons were added to each tested network architecture to evaluate the performance of the artificial neural network. Consequently, the selection of the optimal architecture was based on an iterative trial-and-error process (Panchal et al., 2011).

The stopping criterion for training the ANN was a mean squared error (MSE) value of 10^{-3} $(mol\ kg^{-1})^2$ or lower. After training and the normalized prediction data were completed, denormalization was performed to compare experimental and predicted values based on MSE and R^2 analysis.

Following this, analyzing the network's performance involved evaluating the weights of the artificial neural network. The importance of the input variables during the testing phase was assessed using Garson's method, as described in Equation 1 (Garson, 1991).

$$I_j = \sum_k \left(\frac{|w_{jk}| \times \sum_i |w_{ij}|}{\sum_t |w_{jl}|} \right) \quad (1)$$

where:
I_j: importance of variable j;
w_{jk}: weights of variable j for neuron k;
w_{ij}: weights from hidden layer i to the output;
$\sum_t |w_{jl}|$: total sum of the absolute input weights

This step was crucial for understanding the contribution of each input variable to the network's predictions, as the method calculates the importance of each variable by analyzing the weights of the connections and the activation functions within the network. The method employs a formula that combines the weights of the connections between the input and the hidden layers, and between the hidden layers and the

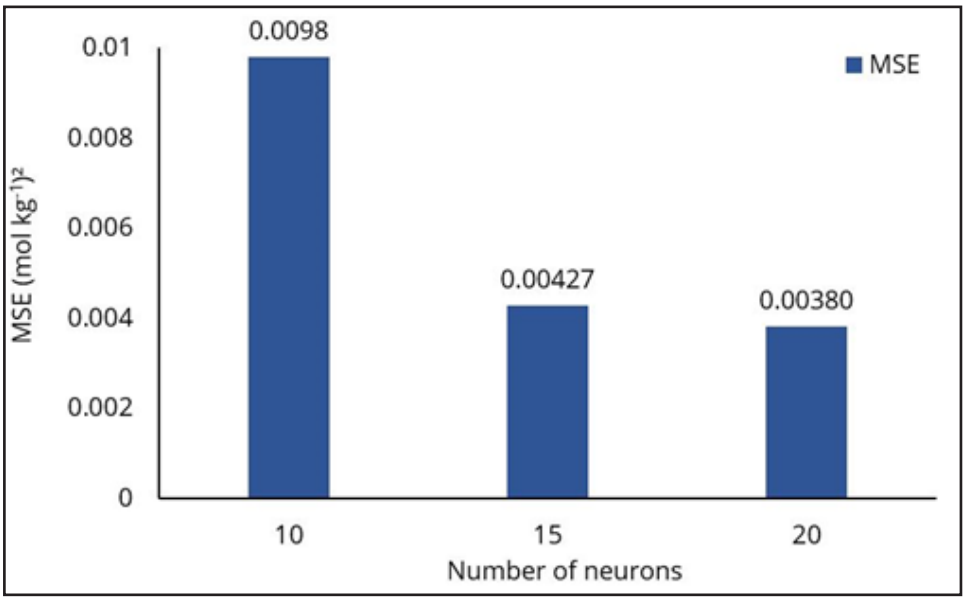
output. The Garson method is valuable for interpreting complex neural networks, providing insights into how input variables influence the model's predictions, and assisting in identifying important variables and reducing dimensionality by removing those with low importance (Garson, 1991).

3 RESULTS AND DISCUSSION

3.1 The artificial neural network

Following the simulation of CO_2 adsorption capacity prediction for a carbon dioxide and methane mixture, the results for MSE and R^2 were systematically recorded in an Excel® spreadsheet for performance analysis of the ANNs. The MSE results were analyzed with the R^2 values to detect potential overfitting. The minimum MSE values obtained for each network architecture tested are presented in Figure 4.

Figure 4 – Comparison of the MSE obtained for each network architecture



Source: Authors (2024)

Analyzing Figure 4, it can be concluded that the ANN architecture with 20 neurons in the hidden layer yielded the lowest MSE. Consequently, this architecture

was selected to present the results of this study. These findings are consistent with other studies on CO_2 adsorption using ANN models, in which variations in the number of neurons in the hidden layer and activation functions have also been explored.

For instance, in a study published by Khoshraftar and Ghaemi (2022), the authors investigated the CO_2 adsorption capacity of activated carbon derived from pistachio shells. They employed an ANN with 30 neurons and the hyperbolic tangent activation function, using pressure, temperature, and adsorption capacity as input variables for the model. After conducting statistical analyses, the network achieved an R^2 of 1 for training, 0.99986 for validation, and 0.99925 for testing, with an MSE of $1.1546x10^{-3}$.

In another study published by Khoshraftar and Ghaemi (2022b), the authors explored the prediction of pure CO_2 adsorption on activated carbon produced from the *Entada Africana* Guill. & Perr. plant using artificial neural networks. The ANN was developed with the Neural Network Toolbox in Matlab, testing architectures with hidden layers ranging from 2 to 20 neurons and employing the hyperbolic tangent activation function. Pressure and temperature were used as input parameters. After statistical analysis, the authors found that the architecture with the best performance had 10 neurons, achieving an R^2 of 0.99977 for training, 0.99985 for validation, and 0.9992 for testing, with an MSE in the range of 10^{-3}.

Rostami et al. (2017) conducted a study on predicting pure CO_2 adsorption on activated carbon using an ANN. The authors utilized the hyperbolic tangent activation function and tested architectures with hidden layers containing 8 to 16 neurons. Pressure and temperature data were used as input variables. Following statistical analysis, they concluded that the architecture with 12 neurons yielded the lowest MSE, at $1.99202x10^{-6}$, and an R^2 of 0.9999.

3.2 Prediction for mono e multicomponent systems

After analyzing the sum of the MSE and R^2 for predicting adsorption capacity, it was observed that at very low pressures ($P < 0.01$ MPa), the simulated

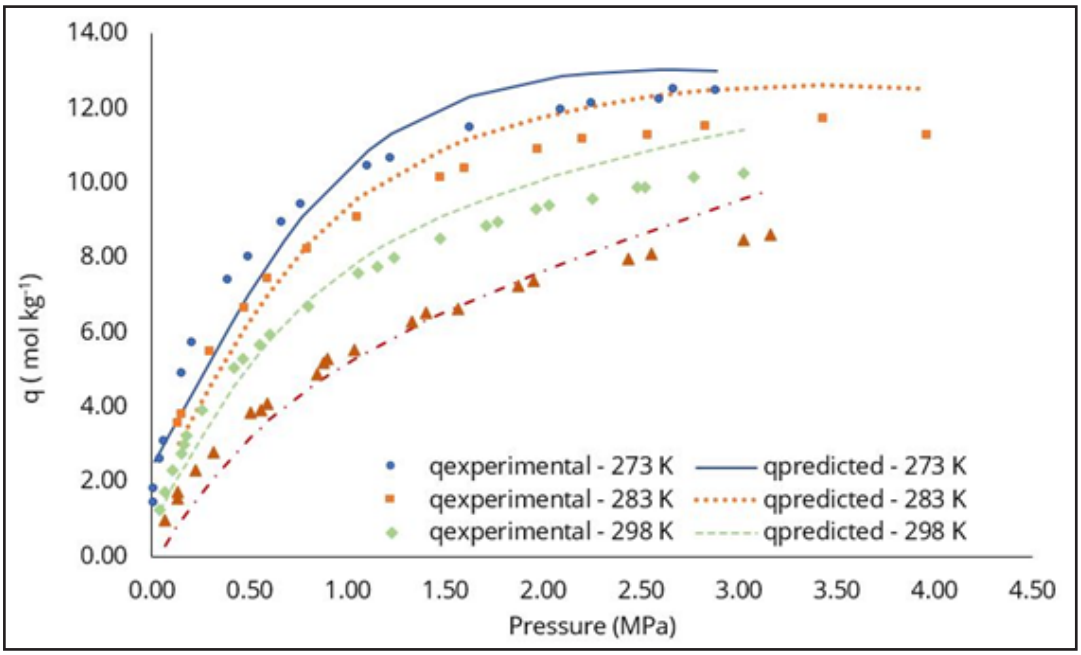
adsorption capacity did not accurately represent the experimental data collected for multicomponent systems.

The influence of pressure on adsorption can often be connected to how the gas density and intermolecular collision frequency decrease. When a system operates at low pressure, the gas behaves more ideally, exhibiting lower density, fewer intermolecular collisions, and alters transport properties such as diffusion and viscosity. These factors must be considered in processes involving gases at low pressures to ensure efficiency and accuracy in industrial and scientific applications (Bird, Stewart, and Lightfoot 2004; Smith et al.2020). Thus, the behavior of gases at pressures approaching zero can influence the gas adsorption process and, consequently, the predictive capability of the ANN for such operating conditions. As a result, data with pressures below 0.01 MPa were excluded to perform a new prediction with the network. For the multicomponent system, a significant reduction in MSE and an increase in R^2 were observed for the CO_2/CH_4 mixture adsorption capacity.

To predict the adsorption equilibrium for pure CO_2, it was necessary to analyze the denormalized data obtained to predict the adsorption capacity. Specific data groups were selected for graphical plotting to demonstrate the behavior of both experimental and simulated data. These data were chosen as they generally represented the data for different temperatures and pressures.

Figure 5 shows the experimental data collected from Himeno, Komatsu, and Fujita (2005) for pure CO_2 at temperatures of 273 K, 283 K, 298 K, and 323 K, with a surface area of 1,450.00 $m^2\ g^{-1}$. Also, the prediction MSE and R^2 data obtained from the ANN model developed in this work are presented in Table 1.

Figure 5 – CO_2 adsorption capacity for a monocomponent adsorption system



Source: Authors (2024)

Table 1 – MSE and R^2 for predicted data of the monocomponent adsorption system

Temperature (K)	MSE	R^2
273	6.8839	0.9744
283	3.8982	0.9915
298	6.1265	0.9874
323	1.5136	0.9969

Source: Organized by the authors (2024)

The analysis of MSE and R^2 shows that the artificial neural network exhibited good predictive capability for the monocomponent system for the adsorbent and the different temperatures used.

For the prediction of the adsorption equilibrium of CO_2 in a multicomponent system, it was necessary to analyze the data resulting from the prediction of CO_2 adsorption capacity in the CO_2/CH_4 mixture at different proportions. Table 2 presents the experimental prediction results for its MSE and correlation coefficient.

Table 2 – MSE and R^2 for predicted data of multicomponent adsorption system

Temperature (K)	MSE	R^2
303.15	45.1190	0.2676
323.15	30.7371	0.0406
353.15	60.7503	0.4042

Source: Organized by the authors (2024)

After analyzing the MSE and R^2 for adsorption capacity prediction, it was noted that for very low pressures ($P < 0.01$ MPa), the simulated adsorption capacity does not represent the experimental data collected for multicomponent systems. Only certain data groups were selected for graphical plotting and table presentation for demonstration purposes. These data were chosen as they generally represented the data for different temperatures and pressures.

Therefore, the data for pressures below 0.01 MPa were excluded to perform a new network prediction for the multicomponent system. The results of the latest prediction are presented in Table 3, in which a significant reduction in MSE and an increase in R^2 for the adsorption capacity of the CO_2/CH_4 mixture were observed.

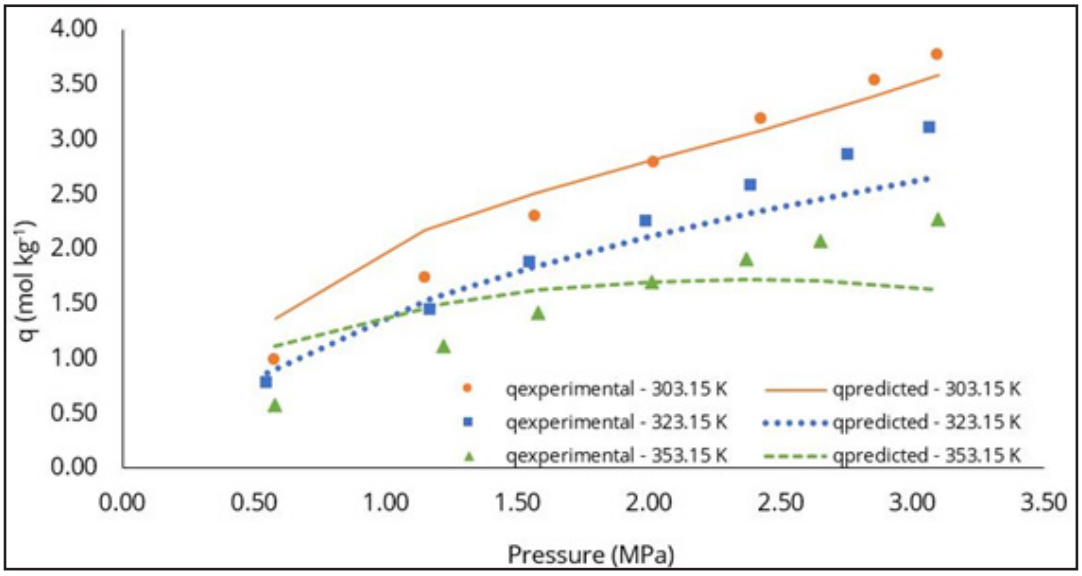
Table 3 – Enhanced MSE and R^2 for the multicomponent adsorption system

Temperature (K)	MSE	R^2
303.15	0.2481	0.9899
323.15	0.2195	0.9887
353.15	0.5309	0.7354

Source: Organized by the authors (2024)

Figure 6 presents a graph showing the second prediction of CO_2 adsorption for the CO_2/CH_4 mixture at temperatures of 303.15 K, 323.15 K, and 353.15 K, using activated carbon with a surface area of 1,290.00 $m^2\ g^{-1}$. The graph includes the predicted data, and the data collected by Pino and Bessieres (2017).

Figure 6 – CO_2 adsorption capacity for the multicomponent system



Source: Authors (2024)

Observing Figure 6 and Table 3, it is apparent that for temperatures of 303.15 K and 323.15 K, the CO_2 adsorption capacity data predicted by the ANN closely match the experimentally obtained data. However, at a temperature of 353.15 K, the CO_2 adsorption capacity data predicted by the ANN show higher MSE and lower R^2 values compared to those obtained at temperatures of 303.15 K and 323.15 K. This difference can be attributed to the limited amount of experimental data collected for the CO_2/CH_4 mixture – only 201 data points, corresponding to 8.34% of the total dataset – which affects its ability to predict data for higher temperatures. Thus, with only 14 input data points available for the temperature of 353.15 K, the prediction of CO_2 adsorption for elevated temperatures may be influenced, potentially resulting in reduced performance by the ANN.

Analyzing the MSE and R^2 data presented in Tables 2 and 3, it was observed a significant reduction in MSE from 45.1190 to 0.2481 for 303.15 K (99.45% reduction), from 30.7371 to 0.2195 for 323.15 K (99.29% reduction), and from 60.7503 to 0.5309 for 353.15 K (99.13% reduction). Also, it was observed an increase in the correlation coefficient from 0.2676 to 0.9899 for 303.15 K (269.92% increase), from 0.0406 to 0.9887 for 323.15 K (143.52% increase), and from 0.4042 to 0.7354 for

353.15 K (81.94% increase). Consequently, the reduction of MSE and increase of R^2 indicates a notable improvement in the prediction of CO_2 adsorption capacity for the multicomponent system.

It can be concluded that the pressure data below 0.01 MPa impacted the ANN's predictive capability for the CO_2/CH_4 mixture, and their exclusion for the new prediction yielded good performance by the ANN, as indicated by the data presented in Tables 2 and 3. Therefore, a potential strategy to further enhance the prediction performance of the ANN is to gather a more representative dataset that accurately reflects the range of input conditions expected during prediction. By ensuring that the dataset covers a broad and evenly distributed variety of input variables, the ANN can be better trained to generalize across different scenarios, leading to more reliable and accurate predictions of CO_2 adsorption capacity in multicomponent systems.

3.3 Importance of variables using Garson's Method

Table 4 presents the weights assigned to each input parameter between the input layer and the network's hidden layer with a 20-neuron architecture.

Each weight reflects the relative importance of each input variable about the activation of a specific neuron in the hidden layer. Higher or lower weight values indicate a variable's impact on the activation of the neuron, which directly influences the final adsorption prediction.

The synaptic weights in the network are adjusted to minimize the discrepancy between the desired output and the actual network output generated by the input signal. The weight of an artificial neuron can span a range that includes both negative and positive values. Positive weights indicate that as the input variable increases, the neuron's activation also increases, contributing to a higher network output. In other words, it directly associates an increase in an input variable with an increase in the adsorption prediction. On the other hand, negative weights indicate that an increase in

the input variable reduces the neuron's activation, leading to a lower network output. This means that, for that neuron, an increase in the input variable is associated with a decrease in the adsorption prediction (Gershenson, 2003; Haykin, 2009).

Table 4 – Weights obtained for the input variables and the hidden layer

Neuron	Pressure	Temperature	Superficial area	qCH_4	qCO_2	q
1	-0.2471	-0.4843	-12.5924	-0.2274	2.1197	3.6982
2	1.9312	-0.2950	0.7497	0.6287	-0.3792	-2.4819
3	1.3997	0.7244	0.1666	-0.2814	1.6569	1.7156
4	1.1894	-1.9573	-1.2905	-1.2209	0.5335	0.6556
5	-2.1763	0.4014	-0.4167	0.1011	-1.2063	0.7859
6	-2.5208	1.6978	-1.1456	-1.2179	-0.8074	-0.3300
7	-1.1238	0.5168	-1.6291	1.4624	-1.1329	-5.4321
8	-0.2398	0.5330	12.4001	-0.0030	-1.8104	3.5474
9	-0.6120	-0.0321	13.2263	2.6100	0.3441	-2.7782
10	-0.8944	-0.0524	-7.3966	0.8431	2.9547	3.2654
11	-2.1265	-0.5535	1.2660	-1.2488	-1.4929	0.6615
12	0.7747	0.1129	-0.1304	0.9178	-0.1764	5.1654
13	-0.1352	0.1019	-12.6408	-0.5038	-2.3644	-2.9988
14	-1.2674	-0.2408	-0.4852	-1.8112	0.5478	2.9619
15	-0.4438	0.3468	-9.1563	2.9895	0.7059	2.7728
16	0.0434	0.1975	-8.8472	1.8309	1.9319	-2.8933
17	5.1408	0.3810	-5.4239	-2.0018	-0.4823	-0.1003
18	-7.7526	-0.6650	-0.3882	1.0756	-0.2909	-4.3153
19	-0.7354	-0.3353	12.5670	-4.2179	-2.3225	7.7897
20	-0.2877	-0.7204	11.4054	-1.4194	-3.5654	-6.4046

Source: Organized by the authors (2024)

The pressure variable shows a weight range between -7.7526 and 1.9312. Pressure has a significant and diverse influence on the network's prediction, as this variable can either increase or decrease the activation of different neurons, depending on the associated weight.

The weight range for temperature varies between -0.7204 and 0.7244, indicating that its influence is more controlled than other variables like pressure and surface area. The surface area shows a weight variation between -12.6408 and 13.2263, suggesting

that this variable plays a key role in adsorption prediction, capable of significantly amplifying or reducing the final output.

The weights for CH_4 adsorption capacity range from -0.7277 to 2.8995, indicating that this variable influences the final prediction. Meanwhile, CO_2 adsorption capacity shows a weight range between -3.5654 and 2.1197, demonstrating a significant that directly affects adsorption prediction.

Therefore, surface area and pressure exert the most significant impact on the ANN's prediction, suggesting that these variables are the most influential in predicting gas adsorption on activated carbon. However, temperature and the adsorption capacities of CO_2 and CH_4 also play important roles, though the range of weights suggests that their influence is more moderate compared to surface area and pressure.

Table 5 presents the weights assigned between the network's hidden and output layers using a 20-neuron architecture. The output weights determine how much each feature the network learns in the hidden layers contributes to the final decision. Therefore, analyzing these weights can reveal which neurons and combinations of input variables are most strongly associated with the model's behavior in the final prediction.

Based on the assigned weights, it was possible to determine the relative importance of the input variables to the network's output variable. To calculate the relative importance, Equation 1 was applied, and the obtained results are presented in Table 6.

It is apparent that the input variables influence the output variable and cannot be ignored in the development of the study. Furthermore, it was concluded that the surface area has the most significant relative importance, while temperature has the least in the adsorption process. Therefore, the input variables incorporated into the network play a crucial role in the network's ability to predict CO_2 capture and should be carefully considered in the study.

Table 5 – Weights obtained for the hidden layer and the output layer

Neuron	Weight
1	4.2900
2	-3.9491
3	-2.6267
4	-3.5471
5	3.3711
6	-2.9196
7	-1.5715
8	-2.6393
9	0.2004
10	-0.2566
11	-0.1846
12	-0.3269
13	2.5471
14	-7.4486
15	1.5916
16	-0.3975
17	7.6415
18	-3.4357
19	-0.1678
20	-3.6370

Source: Organized by the authors (2024)

Table 6 – Relative importance of the input variables

Input Variable	Relative importance (%)
Pressure	12.58
Temperature	9.56
Superficial area	50.06
yCO_2	13.92
yCH_4	13.89
Total	100

Source: Organized by the authors (2024)

4 CONCLUSIONS

The ANN showed good performance in predicting CO_2 adsorption capacity for pure CO_2 without excluding low-pressure data (P < 0.01 MPa). However, when considering low-pressure values, the ANN could have predicted the CO_2/CH_4 mixture more accurately. After excluding data points with pressures below 0.01 MPa, the ANN exhibited good predictive capability for CO_2 capture in the CO_2/CH_4 mix by MSE reduction of 99.45%, 99.29%, and 99.13% and R^2 increasing of 269.92%, 143.52%, and 81.94%. The improved prediction of adsorption capacity for the multicomponent CO_2/CH_4 mixture, following the exclusion of low-pressure data, prompts discussion about the data range used for training the ANN.

The ANN's best prediction of CO_2 adsorption capacity was achieved with 20 layers of neurons, resulting in an MSE equivalent to $3.80x10^{-3}$ and R^2 values of 0.98347 for training, 0.98328 for validation, and 0.97365 for testing. Considering the MSE of order 10^{-3}, correlation coefficients exceeding 0.97 for the employed artificial neural network architecture, and the adsorption equilibrium graphs for experimentally predicted values, it can be affirmed that the use of artificial neural networks is a capable tool for assisting in the prediction of CO_2 capture on commercial activated carbon.

The most important variables identified were surface area (50.06%), molar fraction of CO_2 (13.92%), and molar fraction of CH_4 (13.89%). These variables were crucial in interpreting the influence of input factors on the network's predictions. By analyzing the connection weights and activation functions, Garson's Method provided valuable insights into variable importance, facilitating the identification of key variables and removing less important variables to simplify the model.

The prediction of adsorption capacity using artificial neural networks makes it possible to study the capture of other gases based on experimental data, both for single-component and multicomponent systems. This analysis contributes to the

development of new environmental policies related to carbon emission reduction, allowing for assessing the amount of carbon that can be removed from stationary sources. Consequently, it aids in mitigating the increase in global temperature by facilitating the achievement of the objectives established in the Paris Agreement.

In future studies, several aspects can be further explored to enhance the simulation and prediction of CO_2 adsorption using artificial neural networks (ANNs). One key area for future work involves the selection of input parameters for training ANNs. In addition to the variables already used in this study, such as pressure, temperature, and surface area, other factors like pore size distribution, adsorbent regeneration cycles, or the presence of contaminants, such as water vapor, could provide a more comprehensive model of the adsorption process. Introducing kinetic data, such as adsorption/desorption rates, could also refine the prediction accuracy for dynamic systems.

Regarding computational tools, while this study used MATLAB's Neural Network Toolbox, other machine learning libraries like TensorFlow, PyTorch, or Scikit-learn offer flexibility and scalability for ANN implementation. Additionally, hybrid models combining ANNs, including genetic algorithms or particle swarm optimization, could be developed to optimize the neural network's structure or fine-tune the hyperparameters for improved performance.

Alternative machine learning techniques such as support vector machines (SVM), random forest, or even deep learning models could also be explored to compare performance and accuracy in predicting adsorption behavior. Such comparisons may reveal the strengths or limitations of different methods in modeling complex adsorption systems. SVM can effectively predict CO_2 adsorption capacity, especially when there is a clear separation in adsorption regimes. It can be applied using Support Vector Regression (SVR) to model complex relationships between pressure,

temperature, and surface area variables. Random Forest is helpful for regression in systems with complex and nonlinear interactions, such as CO_2 adsorption in activated carbon. It handles high-dimensional datasets and provides accurate predictions based on multiple input variables.

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