COMMUNICATION

On the Structural Limitations of Neural Networks for Modeling Nonlinear CO_2 Adsorption Equilibria

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Abstract

Machine learning has emerged as a flexible alternative for modeling adsorption equilibrium. However, its limitations in highly nonlinear systems remain unclear. In this work, a feedforward neural network was evaluated using experimental adsorption data for CO_2 and N_2 on zeolite 13X taken from the literature. While the model accurately reproduces N_2 adsorption behavior, it exhibits systematic deviations for CO_2, particularly at higher loadings. Training diagnostics reveal a persistent validation loss plateau, indicating a limitation in the model's ability to further reduce prediction error. These results suggest that the discrepancy is not due to data quality or overfitting, but rather to a structural mismatch between the neural network representation and the strongly nonlinear, saturating nature of CO_2 adsorption. The findings highlight the need for hybrid approaches that incorporate physical structure, such as models based on the Langmuir isotherm.

Keywords: chemical engineering, neural networks, adsorption, carbon capture.

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1 Introduction

The rapid advancement of machine learning techniques, together with significant progress in computational power and data availability, has enabled the development of data-driven models for complex physicochemical systems. These approaches offer attractive alternatives to traditional modeling strategies, particularly when seeking efficient and flexible representations of nonlinear processes. At the same time, the chemical industry faces increasing pressure to address sustainability challenges, including improving energy efficiency, reducing reliance on fossil fuels, and mitigating greenhouse gas emissions. In this context, carbon capture technologies have gained considerable attention, and the application of machine learning to model adsorption processes emerges as a promising strategy.

Adsorption is a complex physicochemical phenomenon governed by multiple variables, including temperature, pressure, and the properties of the adsorbent material. Traditionally, the modeling of adsorption equilibria relies on experimentally derived isotherms and the estimation of parameters associated with established models, such as the Langmuir or Freundlich-type equations, as demonstrated in studies of CO_2 separation on zeolite fixed beds [1].

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While these models provide physically meaningful representations, they require careful selection and calibration for each system. As an alternative, neural networks (NNs) have been proposed as universal function approximators capable of learning adsorption behavior directly from data, potentially bypassing explicit model formulation and enabling their integration into hybrid frameworks for process simulation and control.

However, adsorption systems involving CO_2 are known to exhibit strong nonlinear behavior arising from high affinity interactions and saturation effects [2]. Although neural networks are theoretically capable of approximating arbitrary nonlinear functions, the practical ability of purely data-driven models to capture such structured nonlinearities remains insufficiently understood. In this work, the performance of standard feedforward neural networks is evaluated using experimental adsorption data for CO_2 and N_2 over the same adsorbent material. Despite employing identical inputs, feature engineering strategies, and network architectures, a marked difference in predictive capability is observed. These results reveal inherent structural limitations of purely data-driven neural network models when applied to highly nonlinear adsorption equilibria.

2 Methods

Experimental adsorption data were collected from the studies reported in Yu and Zhan [3, 4], where the adsorbent material was consistently zeolite 13X. The authors provided equilibrium adsorption loadings (q) measured over a range of operating conditions, with temperatures between 303.15 and 363.15 K and pressures spanning from 1 to 174 kPa. To enhance the ability of the neural network to capture the underlying nonlinear behavior of the system, additional input features were constructed from the original variables. Specifically, the natural logarithm of pressure and the inverse of temperature were included as supplementary inputs, providing a transformed representation of the thermodynamic dependencies relevant to adsorption equilibria.

A feedforward neural network was implemented using a fully connected architecture with two hidden layers and nonlinear activation functions. The model receives four input variables — pressure, temperature, logarithmic pressure, and inverse temperature — and produces a single output corresponding to the adsorption loading. To ensure numerical stability and improve convergence during training, both input and output variables were normalized using standard scaling. The dataset was divided into training and validation subsets using a fixed random seed to ensure reproducibility. Model training was carried out using the Adam optimizer with mean squared error as the loss function. Early stopping and learning rate reduction strategies were employed to prevent overfitting and to facilitate convergence. In addition, deterministic settings were enforced throughout the training process by fixing random seeds and controlling sources of stochasticity within the computational framework.

Model performance was evaluated by comparing predicted and experimental adsorption loadings for both CO_2 and N_2 systems. Attention was given to the evolution of the validation loss during training, as well as to the model's ability to reproduce the nonlinear characteristics of the adsorption isotherms across the full pressure range.

3 Results

The performance of the neural network model was evaluated for both CO_2 and N_2 adsorption systems using parity plots and training diagnostics. Figures 1 and 2 present the comparison between predicted and experimental adsorption loadings for CO_2 and N_2, respectively. For the N_2 system, the neural network provides an accurate representation of the adsorption equilibrium across the entire temperature and pressure ranges, with predictions closely aligned along the parity line. This indicates that the selected architecture and input features are sufficient to capture the relatively smooth and weakly nonlinear behavior of N_2 adsorption. In contrast, the model exhibits systematic deviations when applied to CO_2 adsorption data. As shown in Figure 2, the predictions deviate from the parity line, particularly in regions corresponding to intermediate and high loadings. These discrepancies persist despite the inclusion of feature transformations such as logarithmic pressure and inverse temperature, as well as the use of regularization and training stabilization strategies. Further insight into this behavior is provided by the evolution of the training and validation losses, shown in Figure 3. While the model converges rapidly during the initial training stages, the validation loss reaches a plateau and exhibits only marginal improvements thereafter. This behavior suggests that the neural network reaches a limit in its ability to reduce prediction error, even in the absence of overfitting. The observed differences between CO_2 and N_2 can be attributed

to the underlying physicochemical characteristics of the adsorption process. CO_2 adsorption on zeolite 13X is known to exhibit strong nonlinear behavior, characterized by high affinity interactions and pronounced saturation effects. This results in a functional dependence that resembles rational forms typically described by models such as the Langmuir isotherm. In contrast, N_2 adsorption exhibits a more gradual and weakly nonlinear response, which can be more easily approximated by standard neural network architectures.

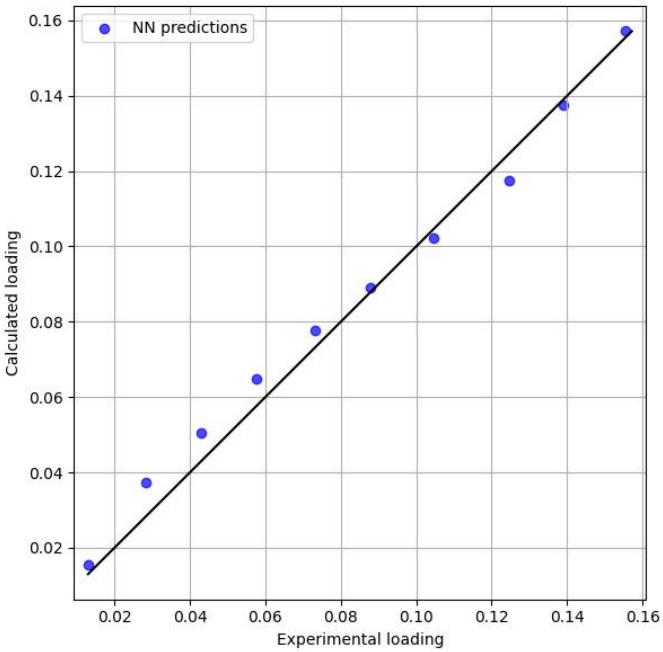

Figure 1. Parity plot between NN predictions and experimental loading for N_2 adsorption.

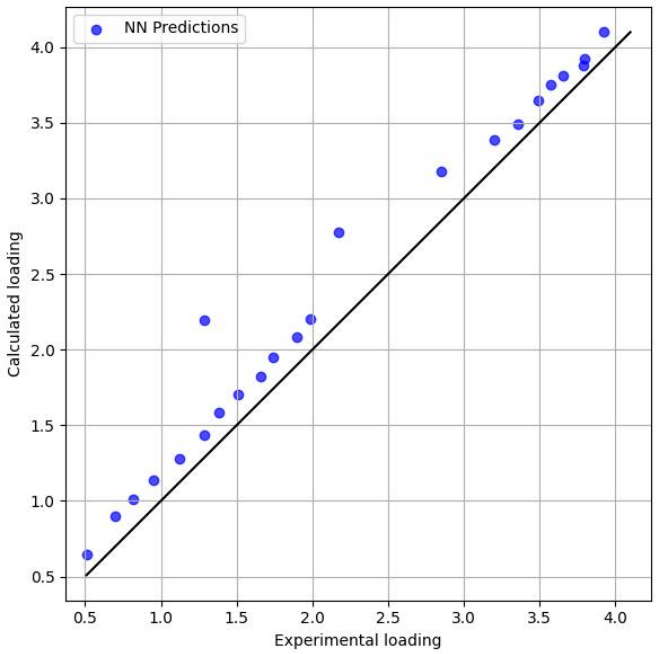

Figure 2. Parity plot between NN predictions and experimental loading for CO_2 adsorption.

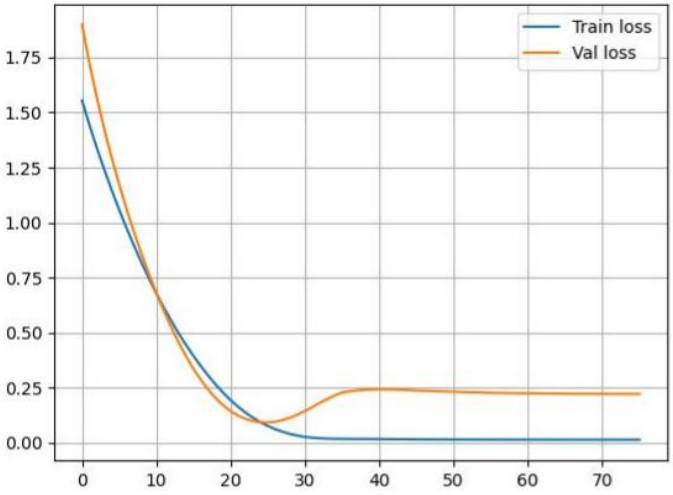

Figure 3. Training and validation loss evolution for CO_2 adsorption.

4 Conclusion

The results of this study demonstrate that standard feedforward neural networks can successfully model adsorption equilibria for systems exhibiting mild nonlinear behavior, as observed in the case of N_2. However, their performance degrades significantly when applied to highly nonlinear systems such as CO_2 adsorption, even when using experimental data from the same adsorbent and incorporating feature engineering strategies. The presence of a persistent validation loss plateau, together with systematic deviations in parity plots, indicates that these limitations are not related to data quality, model training, or overfitting. Instead, they arise from a structural mismatch between the functional representation provided by neural networks and the intrinsic behavior of strongly nonlinear adsorption equilibria. These findings highlight the need for incorporating physical structure into data-driven modeling approaches for adsorption systems. Hybrid methodologies, where neural networks are used in conjunction with physically motivated models such as the Langmuir isotherm, offer a promising direction to overcome these limitations. Such approaches can leverage the flexibility of machine learning while preserving the interpretability and robustness of classical thermodynamic models.

Data Availability Statement

Not applicable.

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Conflicts of Interest

Cristian J. Calderon served as an Associate Editor of the *Journal of Chemical Engineering and Renewable Fuels* at the time of manuscript submission. To ensure the integrity of the peer-review process, Cristian J. Calderon was not involved in the editorial handling, peer review, or decision-making process for this manuscript, which was handled independently by another editor. The remaining author declares no conflicts of interest.

AI Use Statement

The authors declare that no generative AI was used in the preparation of this manuscript.

Ethical Approval and Consent to Participate

Not applicable.

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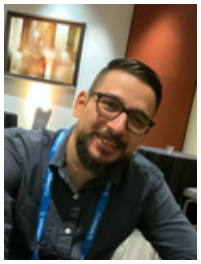

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